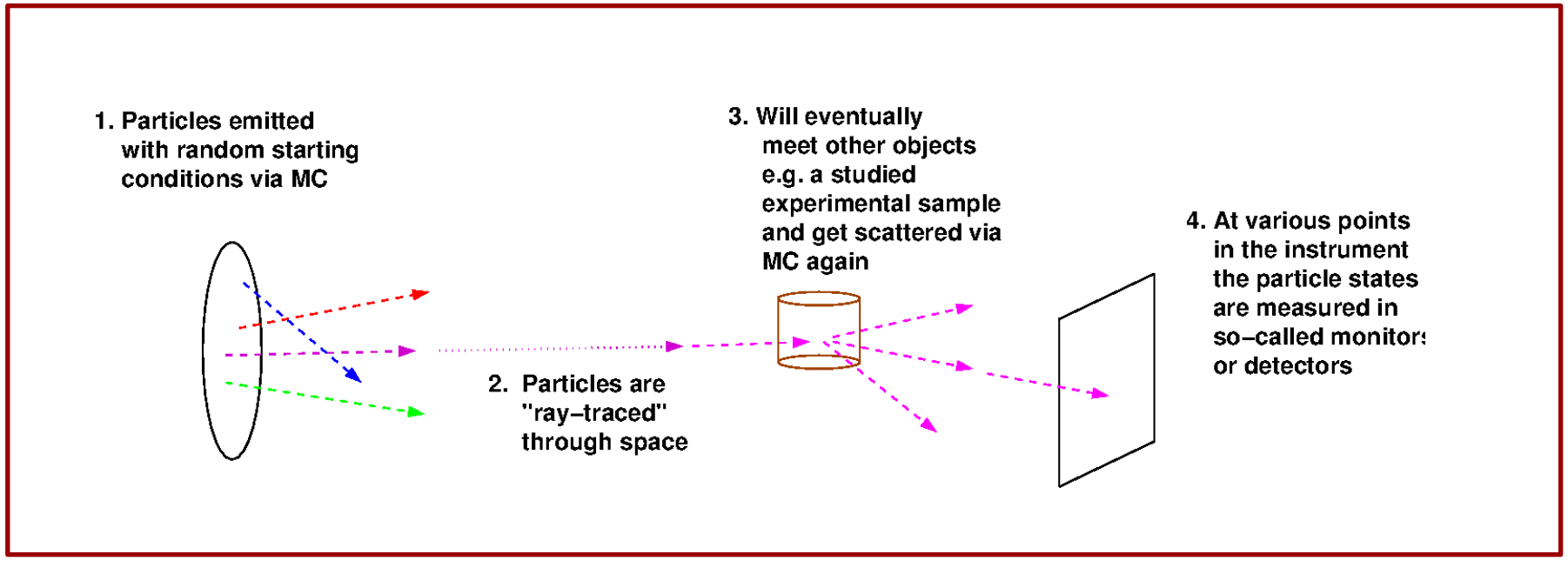
McStas Introduction and general concepts

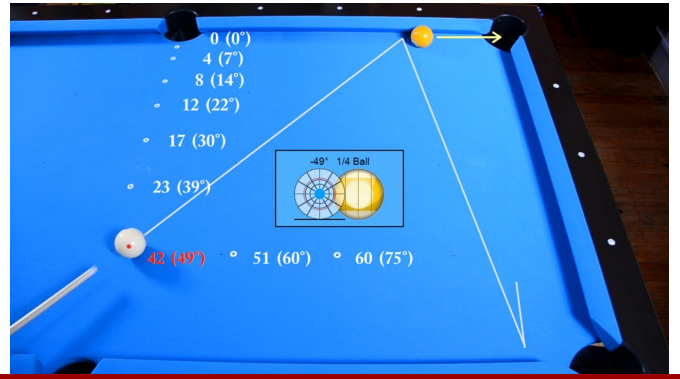
Agenda

- A (very) brief introduction to McStas
- Components of neutron instruments
- How McStas works under the hood
- Components and instruments
- A demo

In the big picture, McStas is this…



- Classical Newtonian mechanics, i.e.



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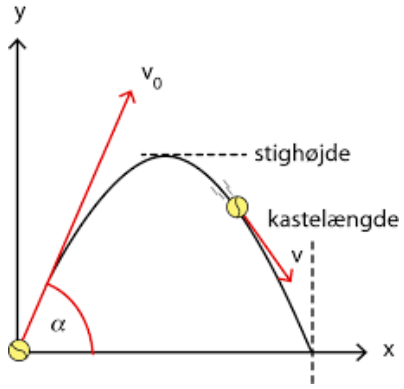

- (independent, particles though…)

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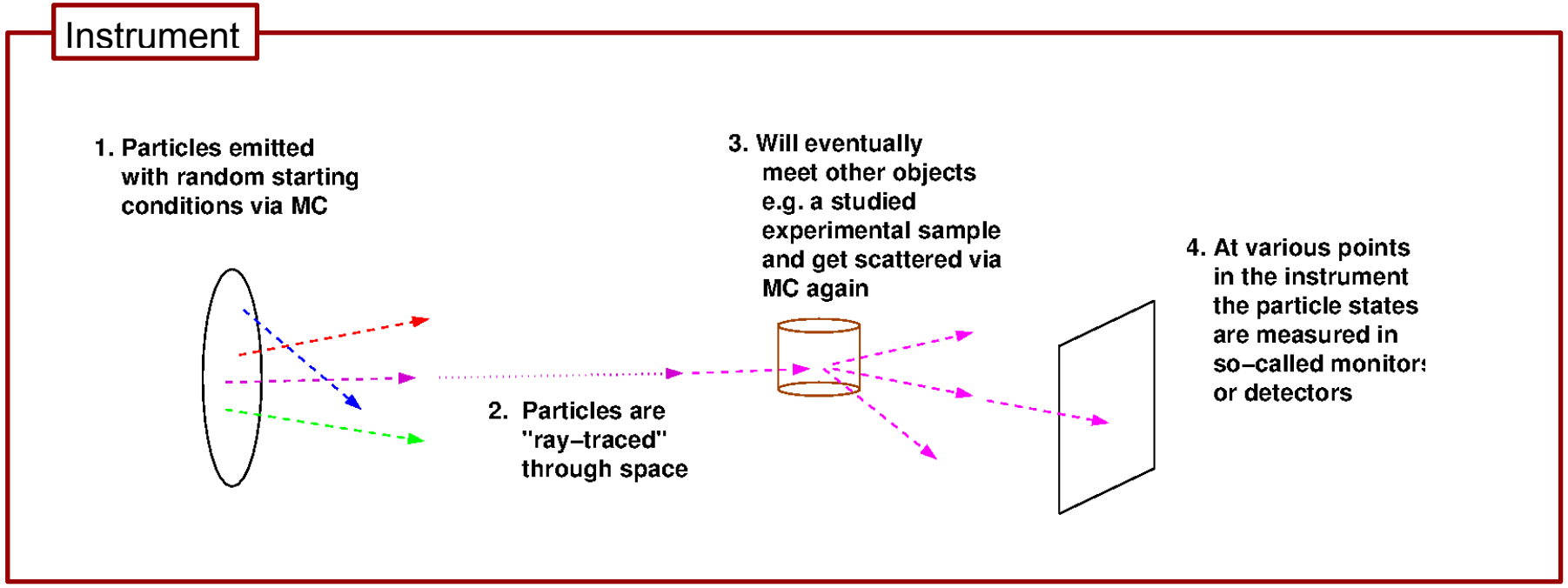
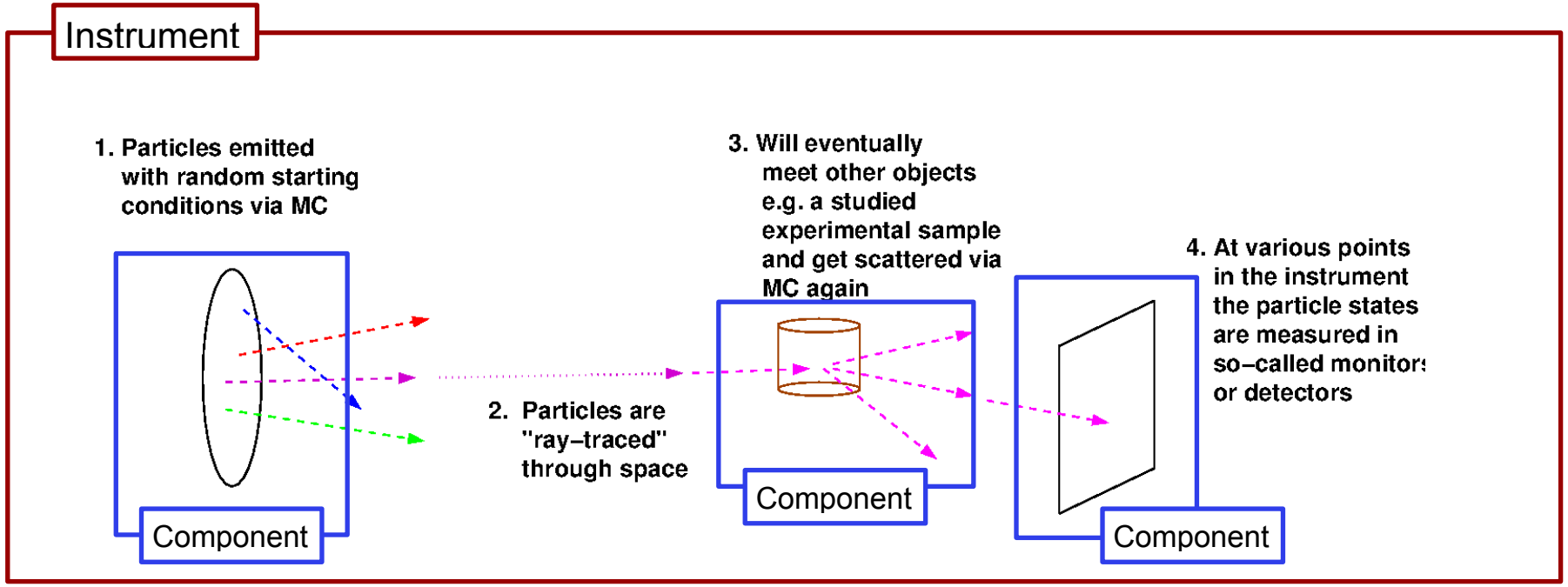


The instrument defines our “lab coordinate system”

In the big picture, McStas is this…



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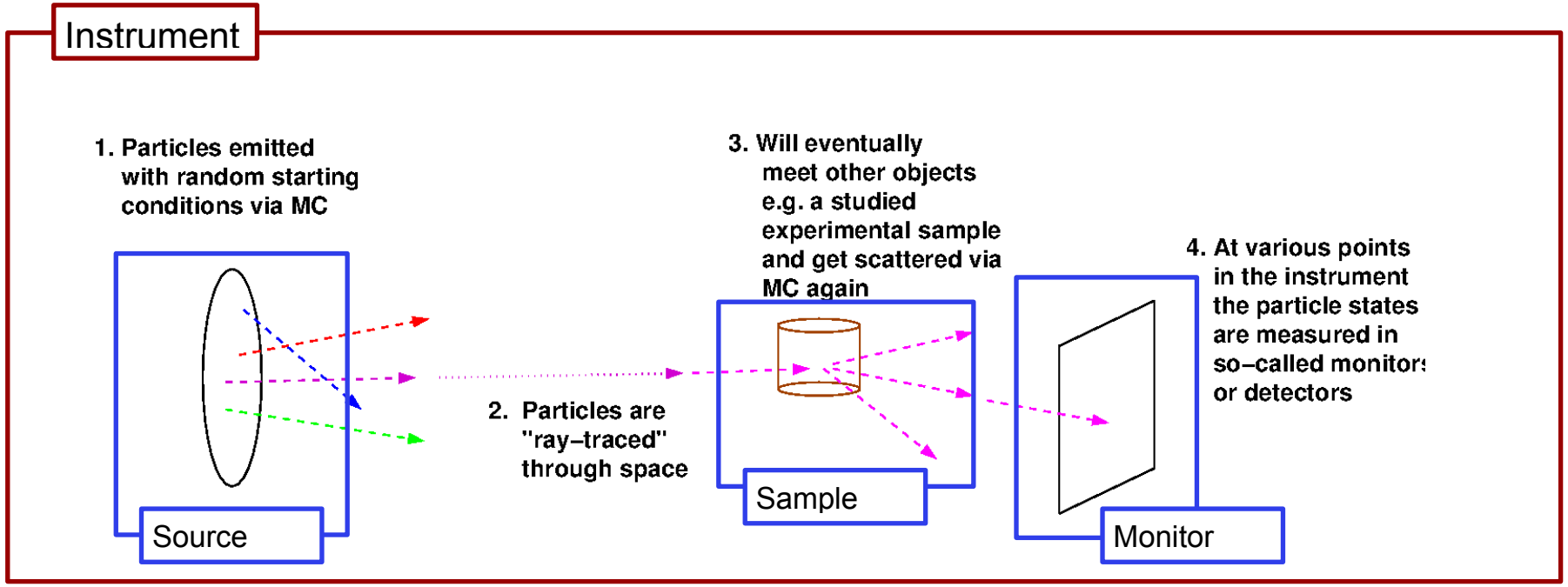
The components define devices or features available in our instrument

In the big picture, McStas is this…



The instrument defines our “lab coordinate system”

The components define devices or features available in our instrument - they have different function

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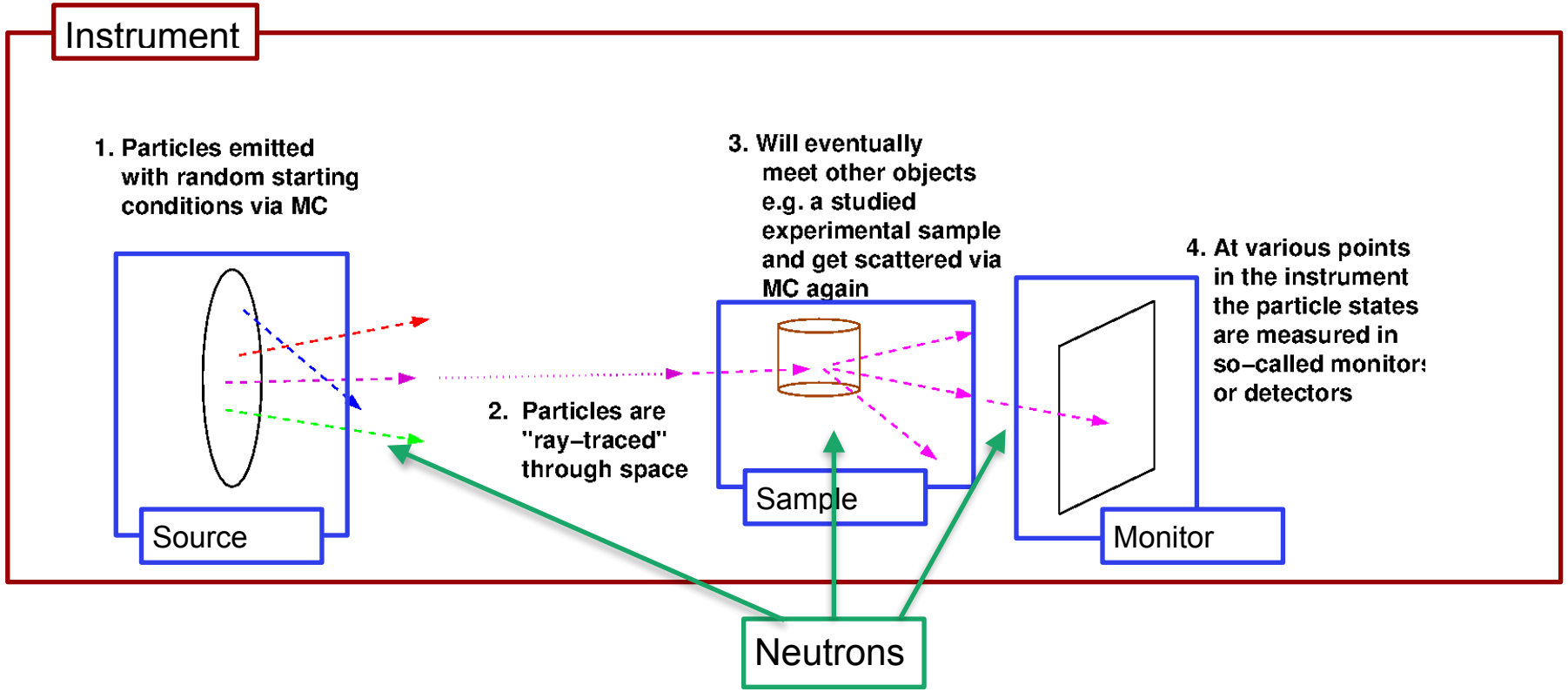
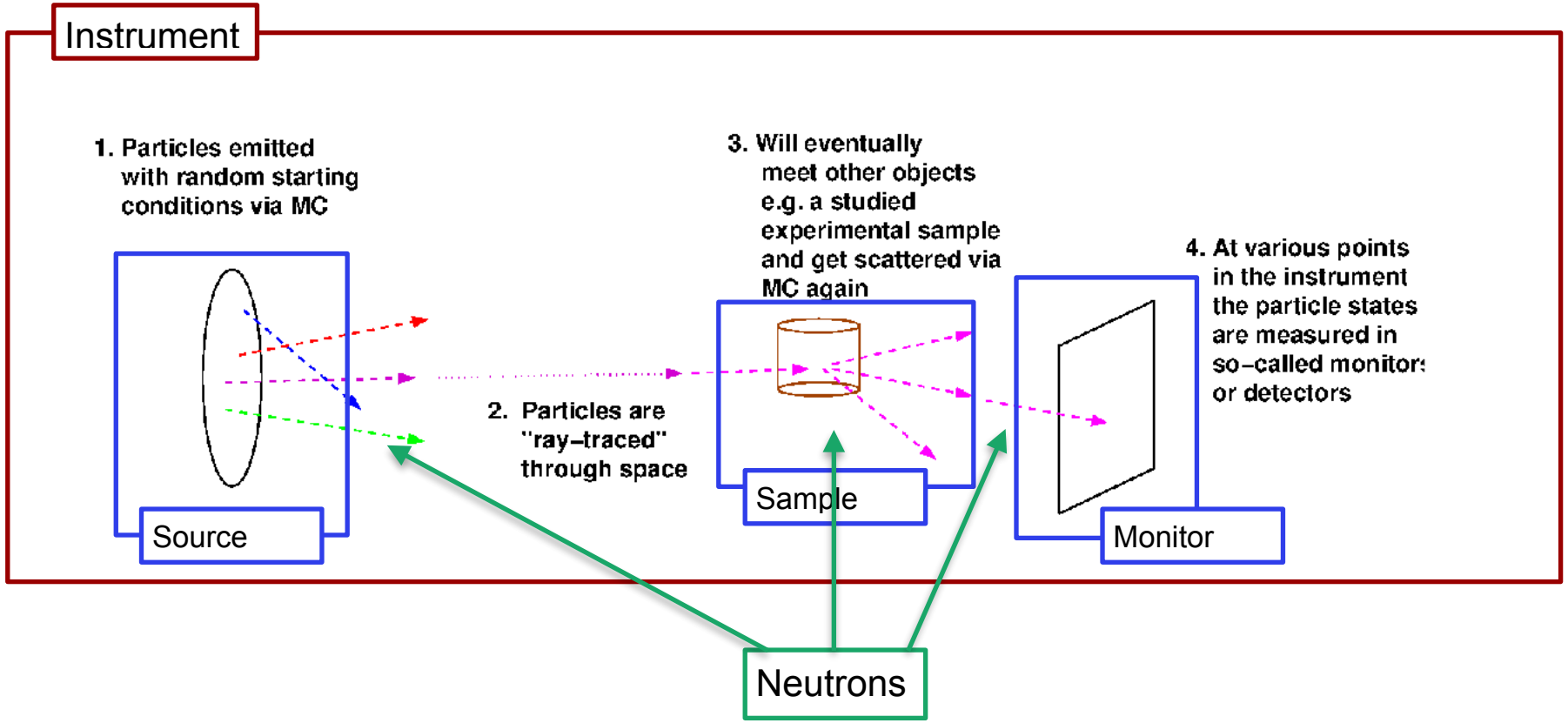


The instrument defines our “lab coordinate system”

The components define devices or features available in our instrument - they have different function

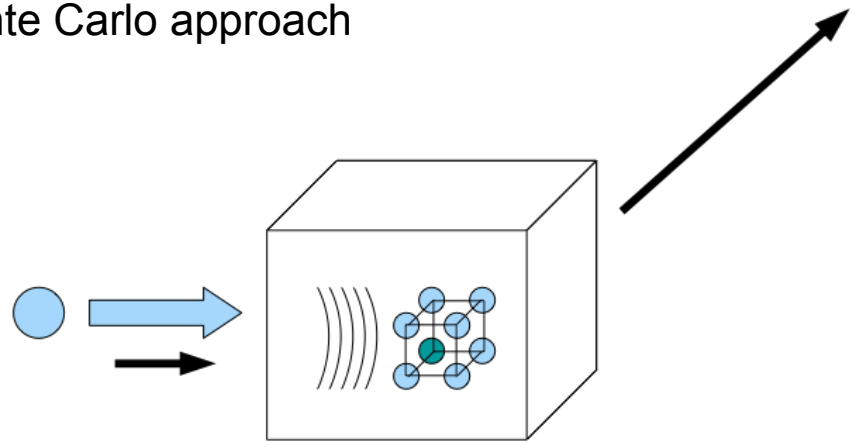
Neutron particles are passed on from one component to the next, changing state under way

McStas is a Monte Carlo ray-tracer



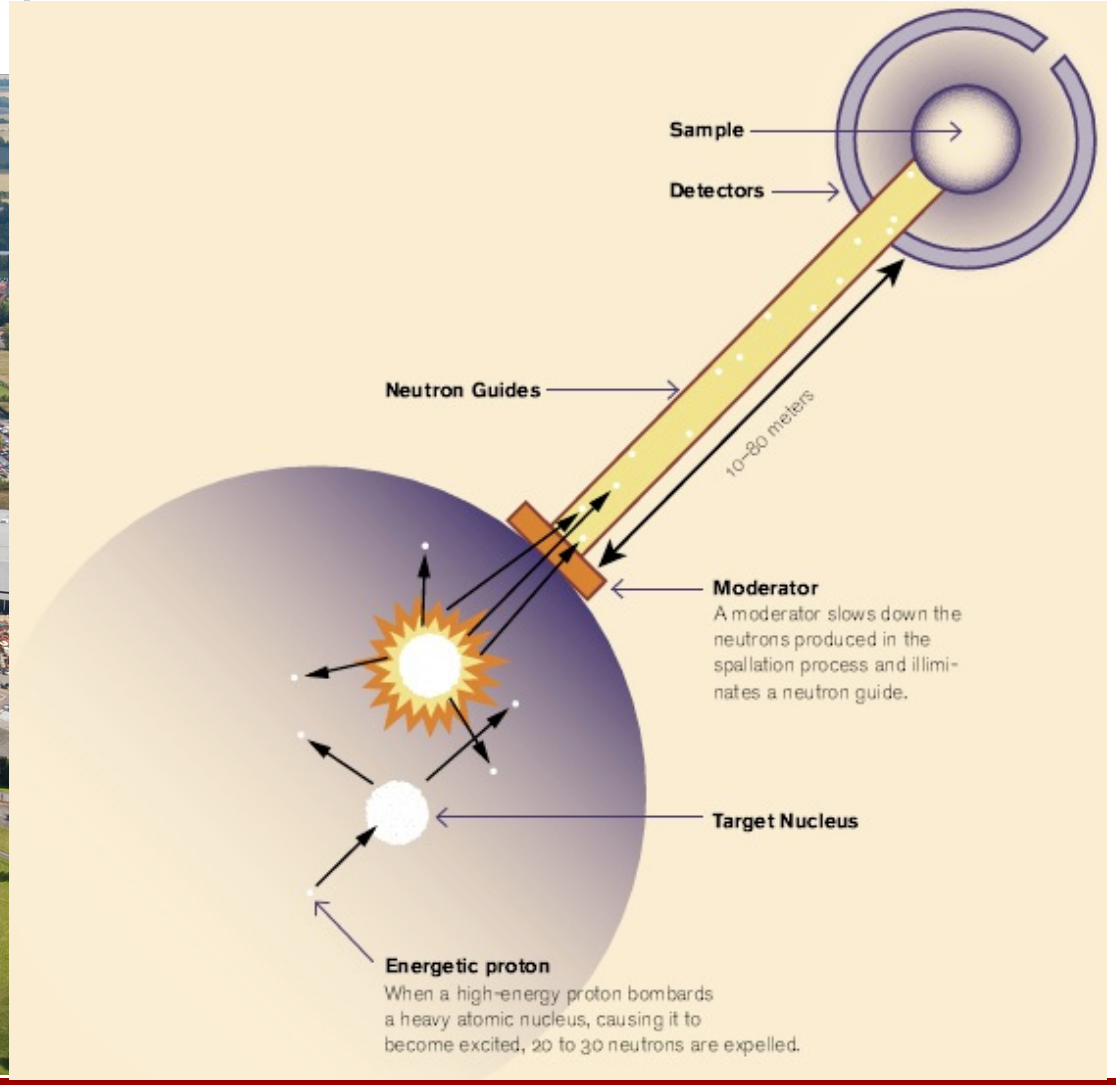
Elements of Monte-Carlo raytracing

- Instrument Monte Carlo methods implement coherent scattering effects
- Uses deterministic propagation where this can be done
- Uses Monte Carlo sampling of “complicated” distributions and stochastic processes and multiple outcomes with known probabilities are involved
- - I.e. inside scattering matter
- Uses the particle-wave duality of the neutron to switch back and forward between deterministic ray tracing and Monte Carlo approach



- Result: A realistic and efficient transport of neutrons in the thermal and cold range

Components of neutron instruments



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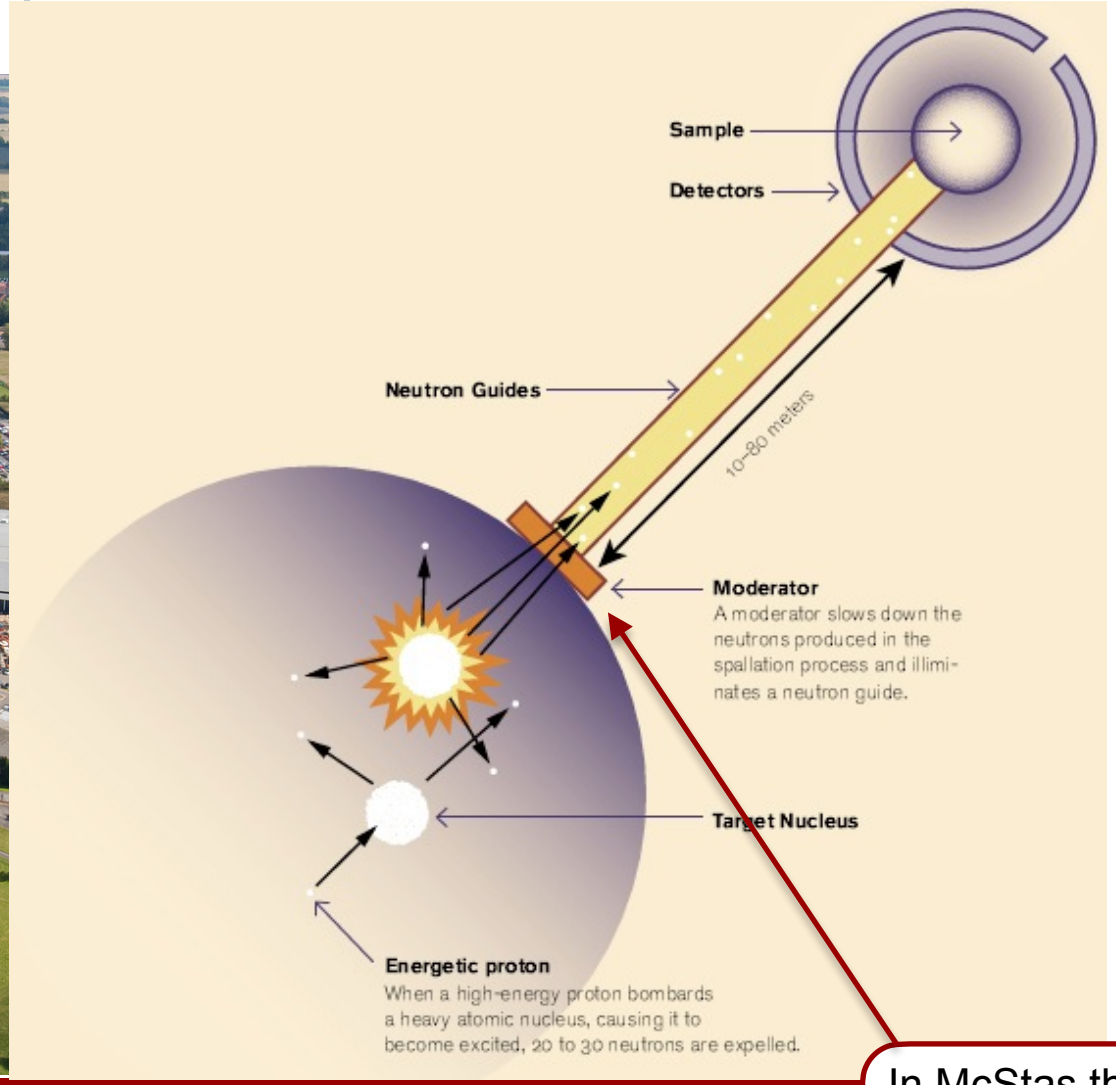
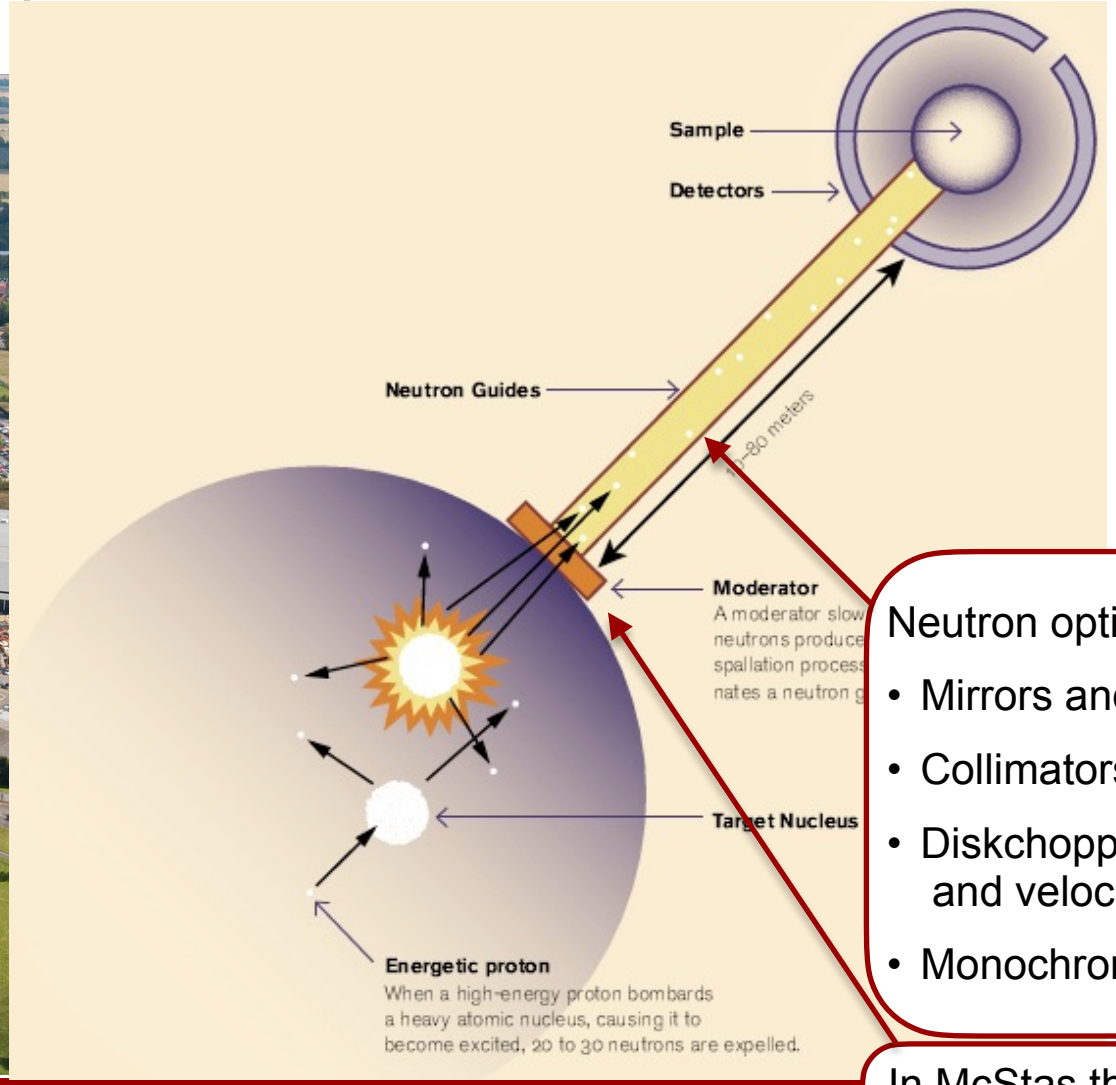


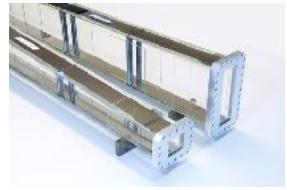
In McStas the moderator is the “source”

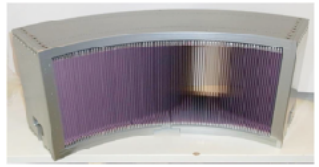
Components of neutron instruments

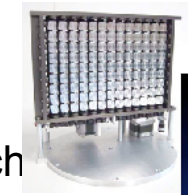


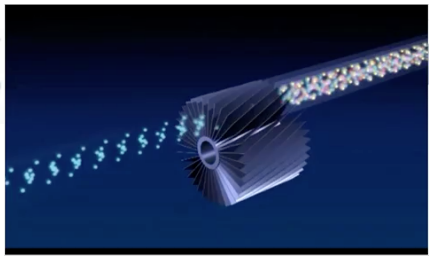
Neutron optics include things like:

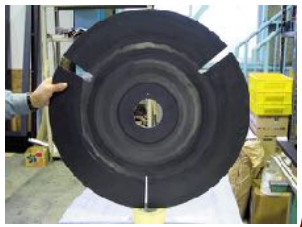
- Mirrors and guides
- Collimators and slits
- Diskchoppers, Fermi ch
  and velocity selectors
- Monochromators/Analysers





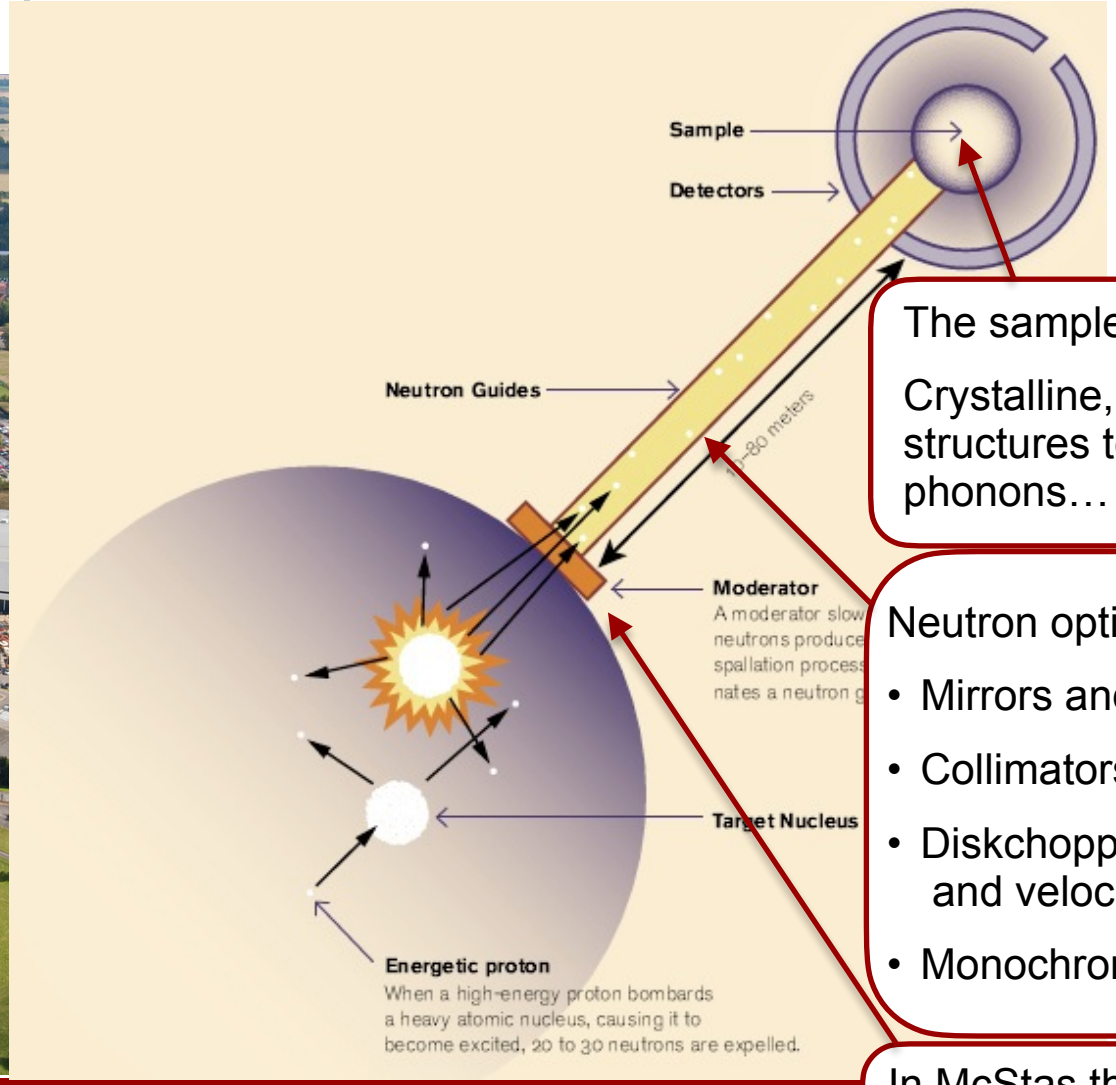






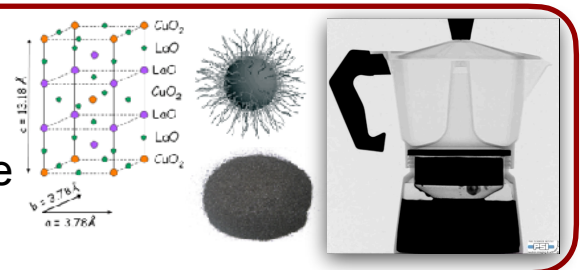
In McStas the moderator is the “source”

Components of neutron instruments



The sample:

Crystalline, powders, liquids, micelles, structures to image, inelastic features like phonons…



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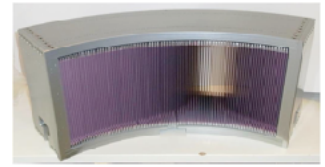

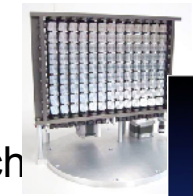

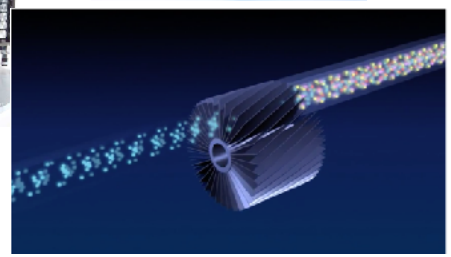

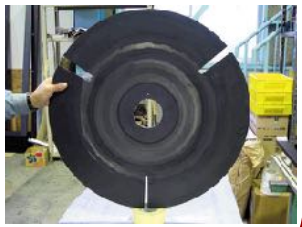

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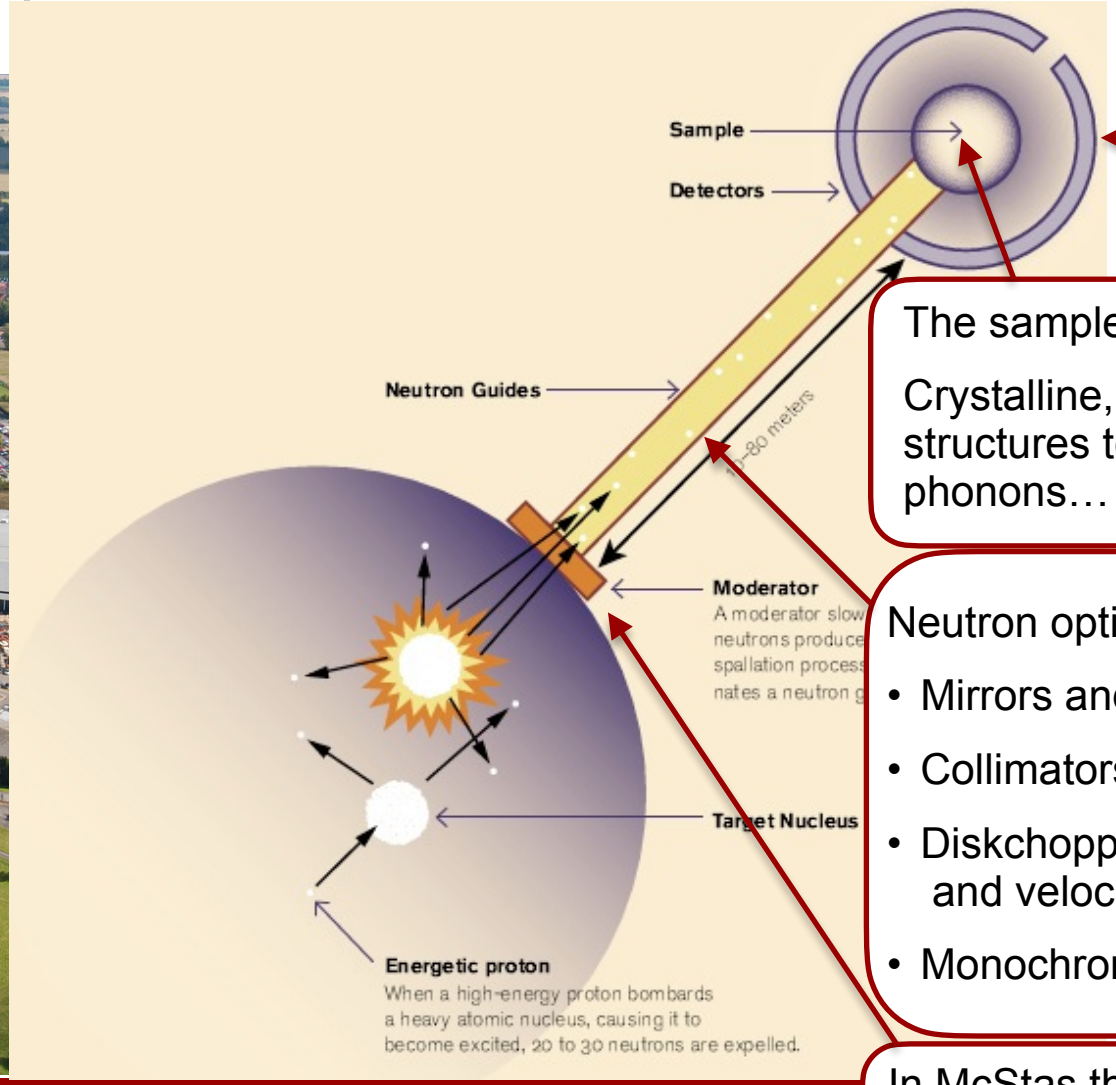
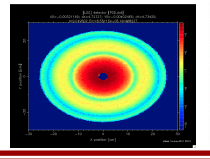
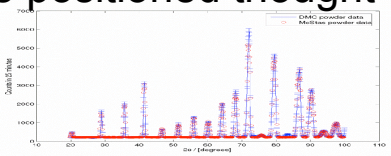
Components of neutron instruments



Detectors are “monitors” in McStas. Mostly they act as “perfect probes” and can be positioned thought your instrument gathering 1D/2D/ event lists…





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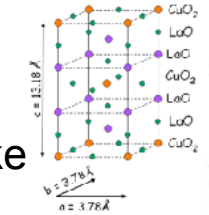

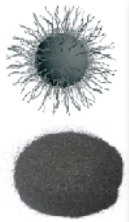

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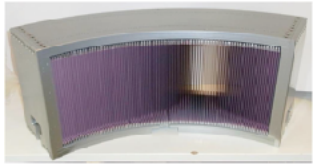

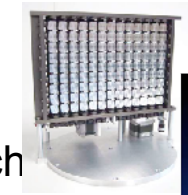

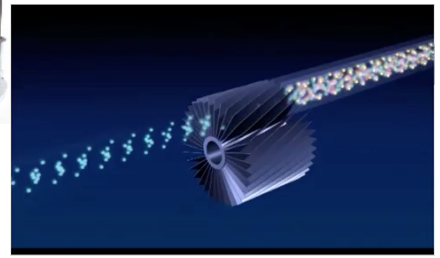

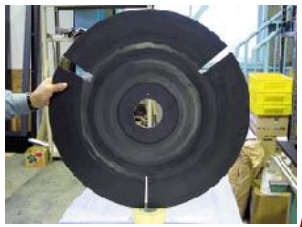

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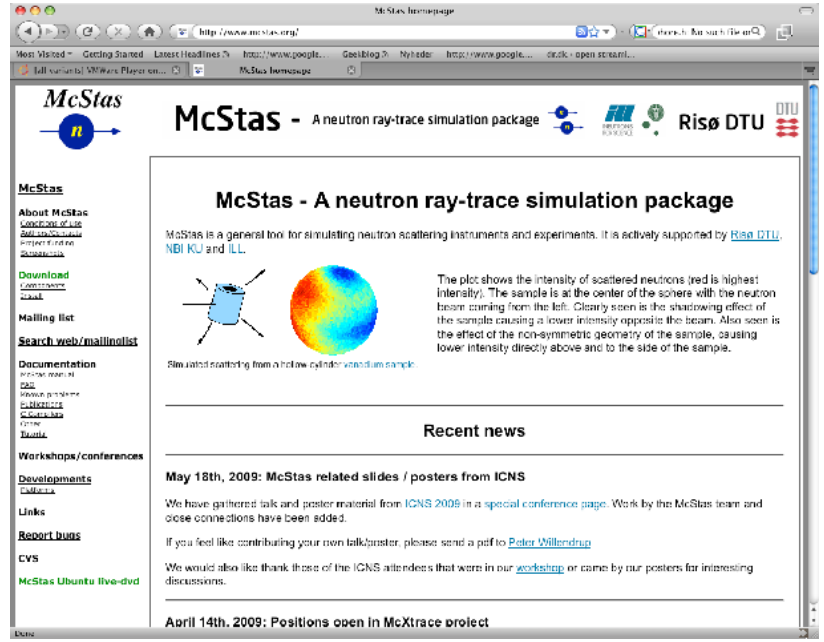
McStas Introduction

GNU GPL license

Open Source

- Flexible, general simulation utility for neutron scattering experiments.
- Original design for Monte carlo Simulation of triple axis spectrometers
- Developed at DTU Physics, ILL, PSI, Uni CPH, ESS DMSC
- V. 1.0 by K Nielsen & K Lefmann (1998) RISØ
- Currently 2.5+1 people full time plus students



Project website at

http://www.mcstas.org

mcstas-users@mcstas.org mailinglist

McXtrace - since jan 2009 similar for X-rays

Main Page – McXtraceWiki

http://www.mcxtrace.org/index.php?title=Main_Page

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McXtrace

Main Page

McXtrace [edit]

McXtrace - Monte Carlo Xray ray-tracing is a joint venture by

Risø DTU DTU ESRF JJ X-RAY

Funding from NABIIT, DSF and the above parties.

Our code will be based on technology from McStas.

For information on our progress, please subscribe to our user mailinglist.

mailto:webmaster@mcxtrace.org

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- Project Goal
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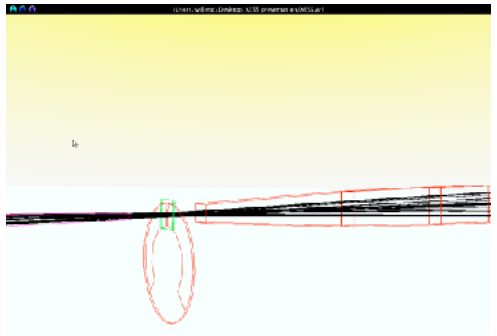
Done

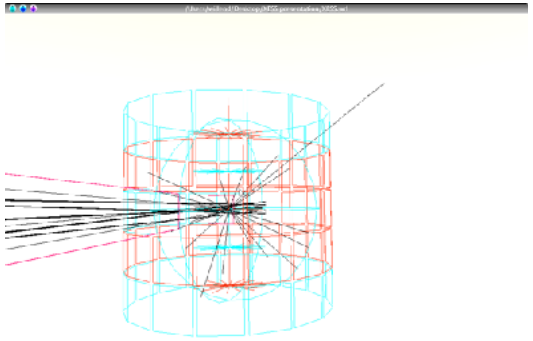
- Synergy, knowledge transfer, shared infrastructure

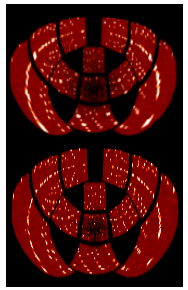
Used in many places

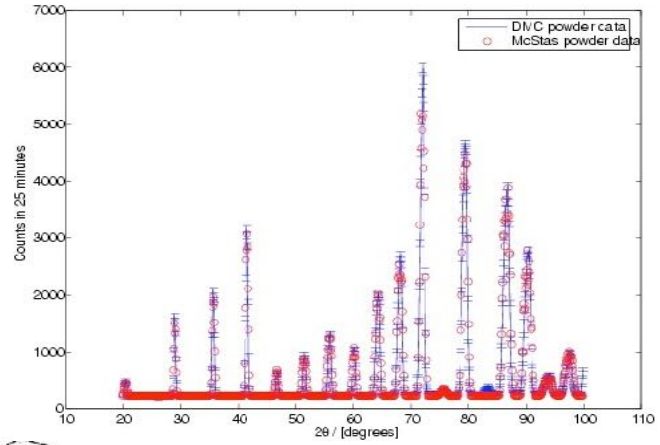
What is McStas used for?

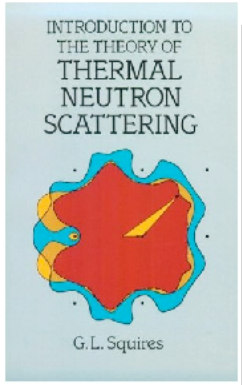
- Instrumentation
- Planning
- Construction
- Virtual experiments
- Data analysis
- Teaching
  (KU, DTU)

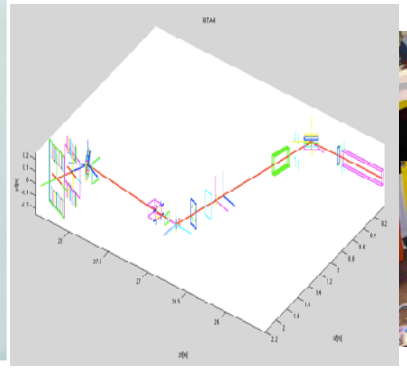


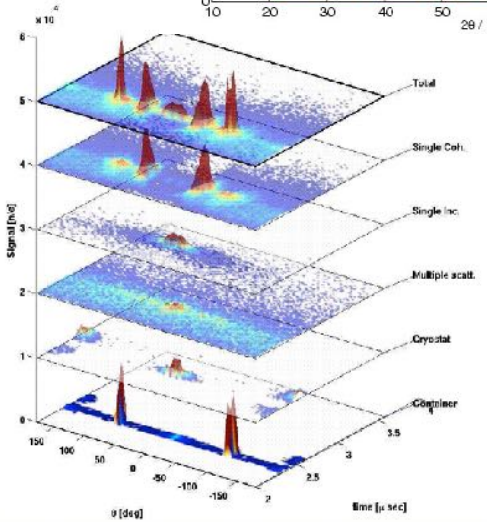






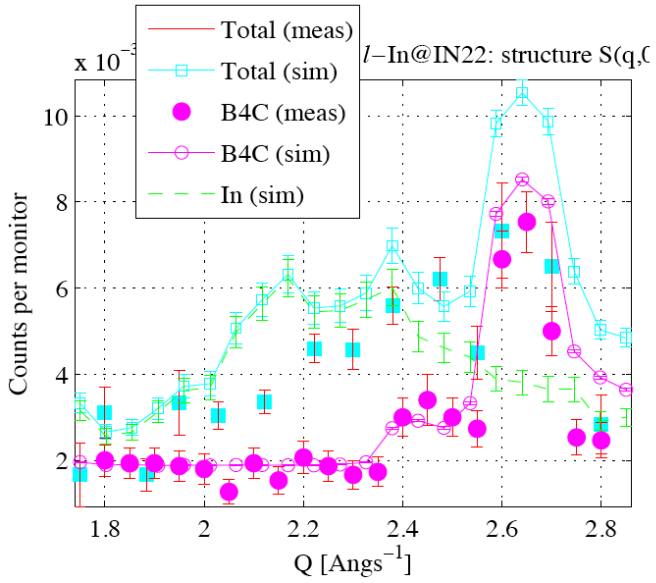




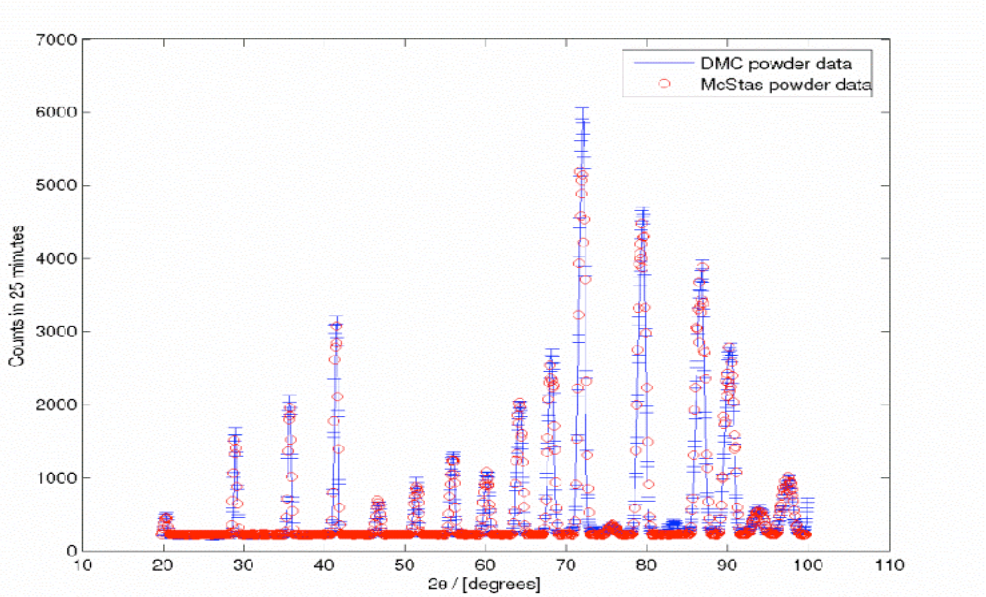


Reliability - cross comparisons

- Much effort has gone into this
- Here: simulations vs. exp. at powder diffract. DMC, PSI
- The bottom line is
- McStas agree very well with other packages (NISP, Vitess, IDEAS, RESTRAX, ...)
- Experimental line shapes are within 5%
- Absolute intensities are within 10%
- Common understanding: McStas and similar codes are reliable



E. Farhi, P. Willendrup



P. Willendrup et al., Physica B, 386, (2006), 1032.

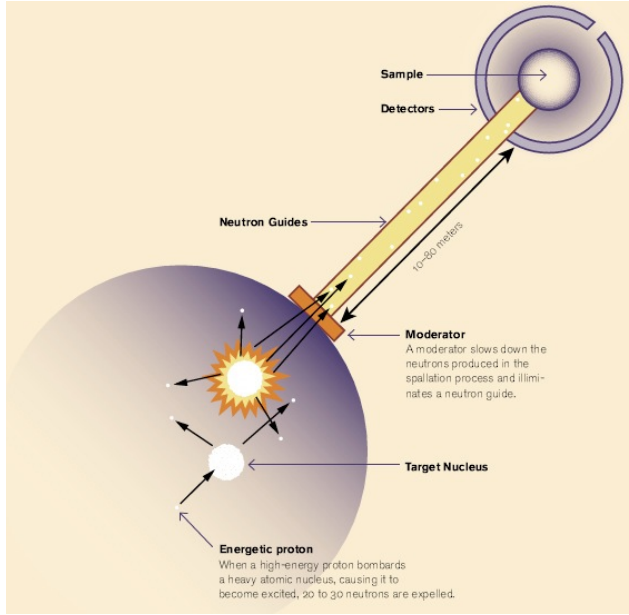
McStas overview

- Portable code (Unix/Linux/Mac/Windoze)

- Ran on everything from iPhone to 1000+ node cluster!

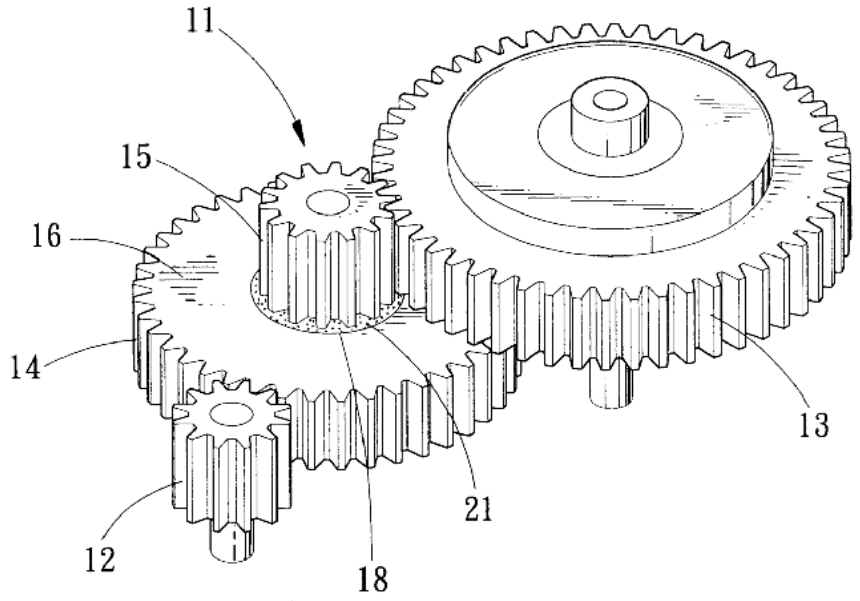
- 'Component' files (~100) inserted from library
  - Sources
  - Optics
  - Samples
  - Monitors
  - If needed, write your own comps

- DSL + ISO-C code gen.



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
  - ...

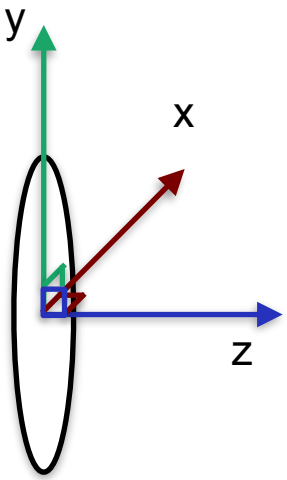


Implementation

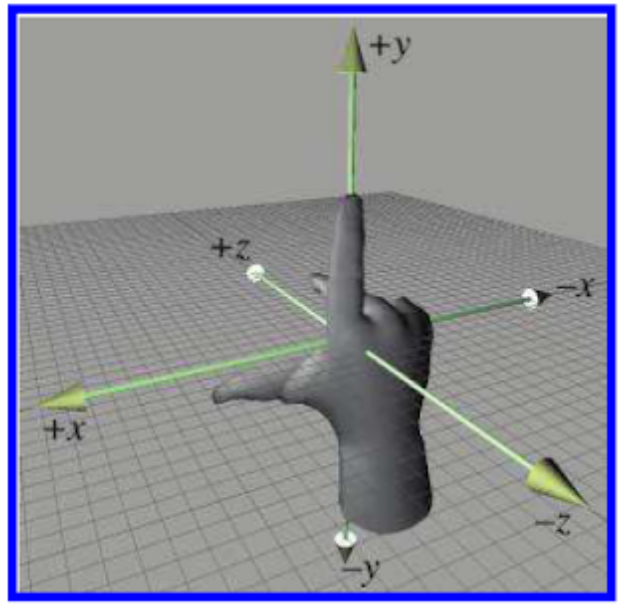
- Three levels of source code:
  - Instrument file (All users)
  - Component files (Some users)
  - ANSI c code (no users)

Placing components - source

- One of the first components in your instrument is typically a source, which has a coordinate system like this….



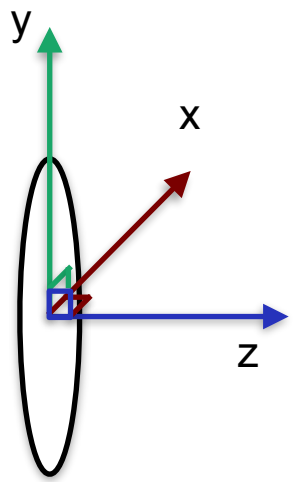
- z is along neutron beam direction
- y is vertical
- x at an angle of 90° wrt. z,y



Right-handed coordinate system

Placing components - source

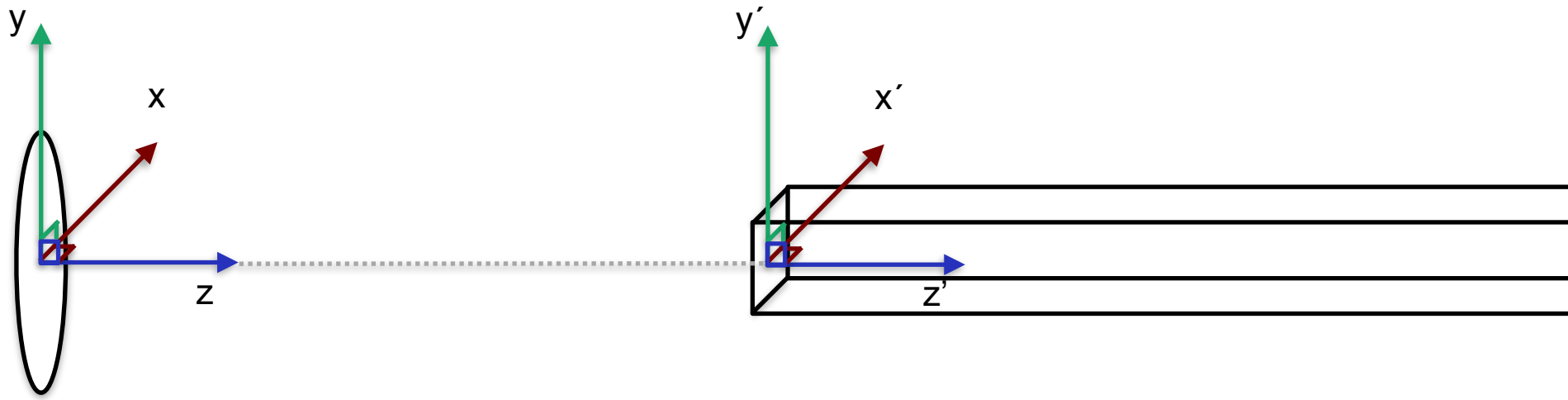
- Often the source coordinate system coincides with the “lab” coordinate system, denoted ABSOLUTE in McStas language, i.e.



- COMPONENT Source = Source_simple(…)
  AT (0,0,0) ABSOLUTE

Placing further components - RELATIVE

Placing further components is done by order of
1. **Location, i.e**

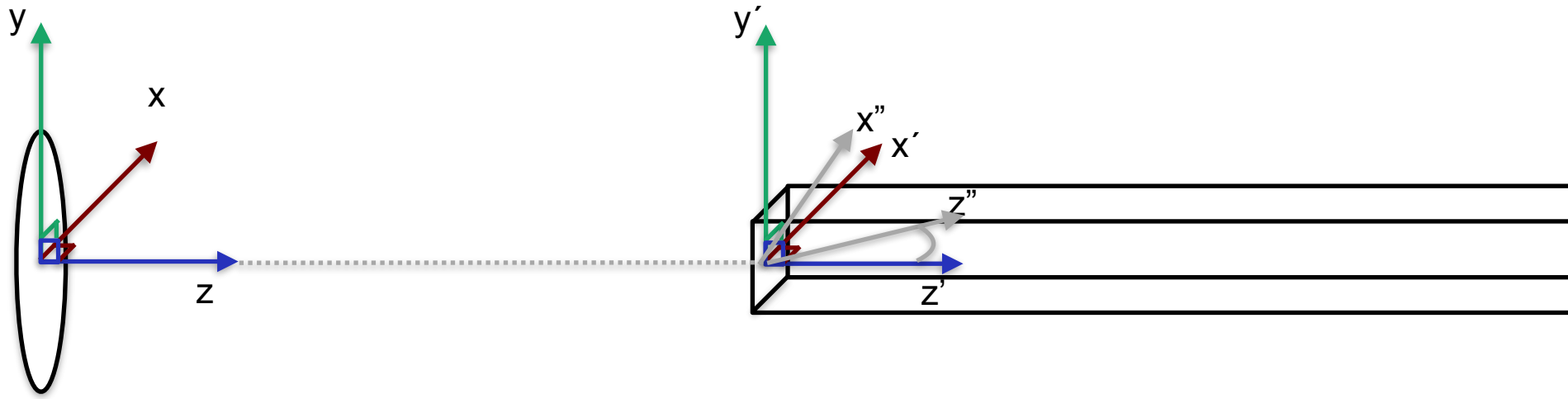


COMPONENT Source = Source_simple(…)
AT (0,0,0) ABSOLUTE

COMPONENT Guide = Guide(…)
AT (0,0,1) RELATIVE Source

Placing further components - RELATIVE

Placing further components is done by order of
2. **Rotation, i.e**

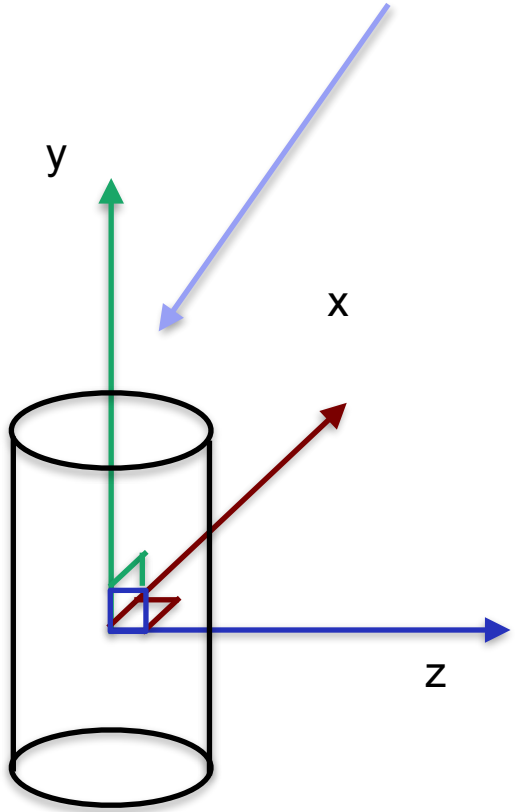


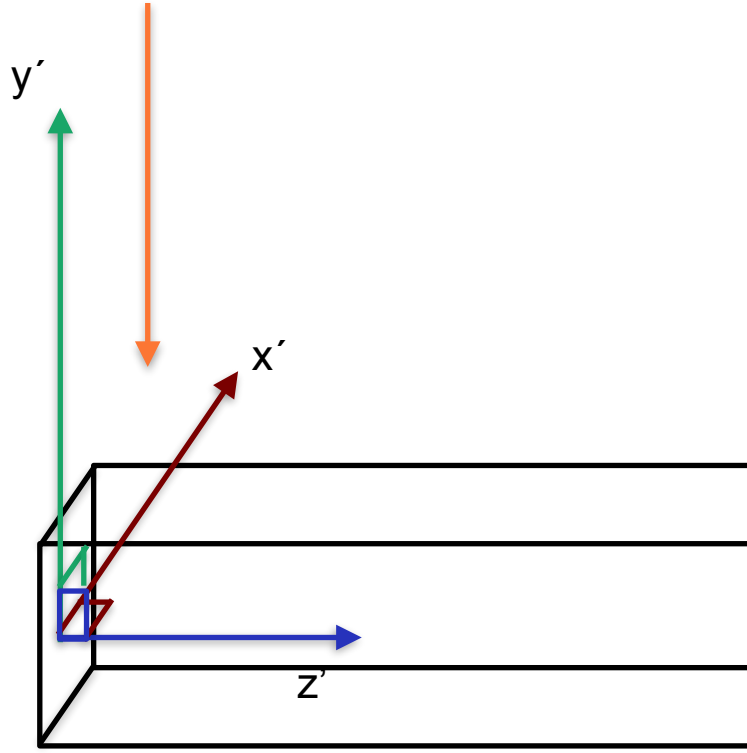
COMPONENT Source = Source_simple(…)
AT (0,0,0) ABSOLUTE

COMPONENT Guide = Guide(…)
AT (0,0,1) RELATIVE Source
ROTATED (0,30,0) RELATIVE Source

(Reference labels can also be PREVIOUS or PREVIOUS+1 etc.)

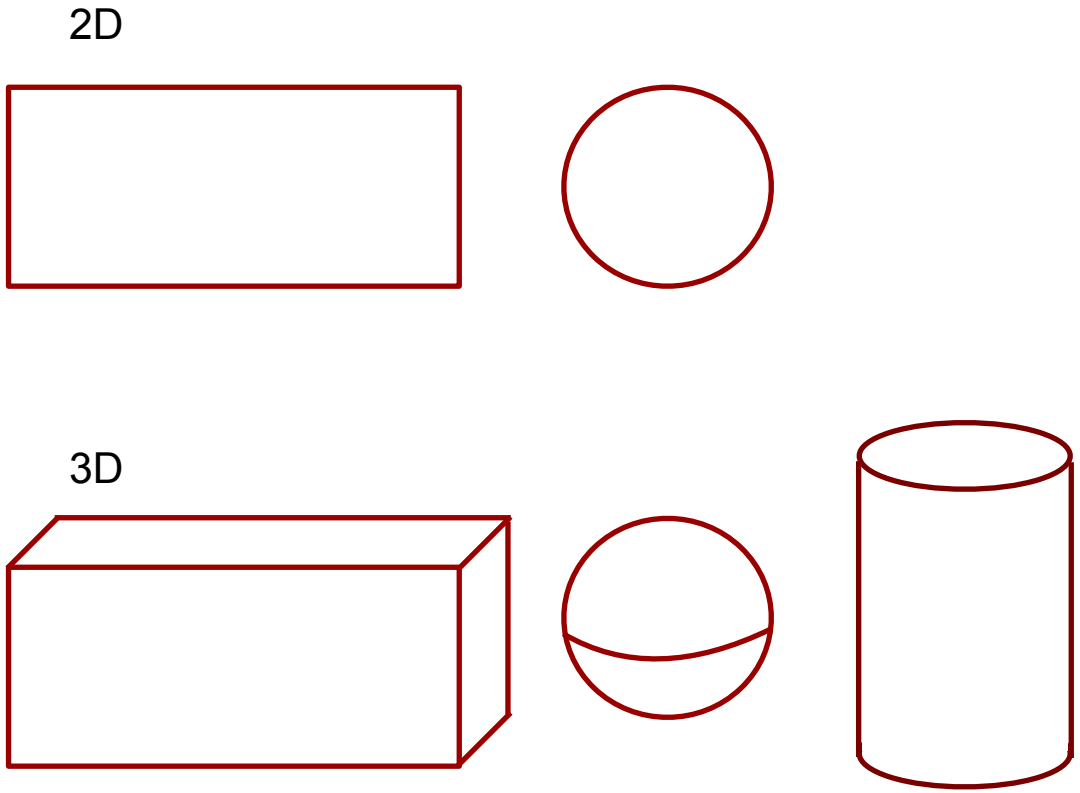
Components often have their origin at the centre of mass, i.e. for samples … but not for neutron guides

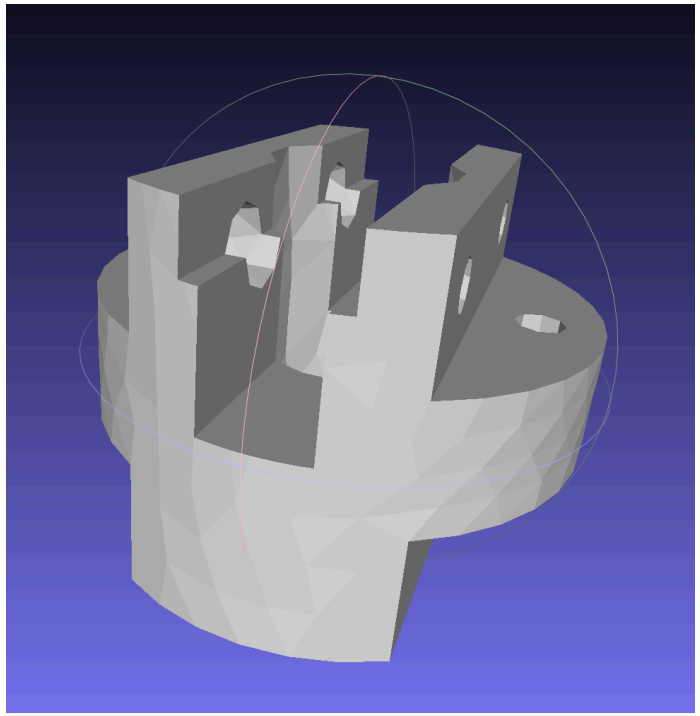




Generally speaking, the component author can choose
the meaningful coordinate system for the given problem!
- The McStas system takes care of the transformation between them….

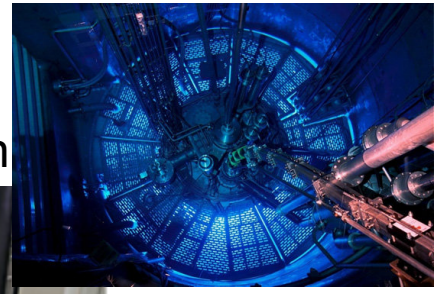
Component geometries are typically simple objects…
But some have polygon-description of the surface





Component classes

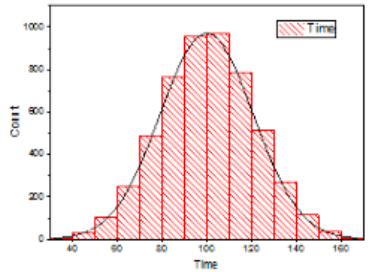
- Sources - these define MC starting conditions / “inject” neutrons to our simulation



- Optics - used to tailor properties of the neutron beam
  - Examples are mirrors, guides, choppers, collimators, slits, …

- Samples - “matter” of some form
  - Powders, single crystals, liquids, micelles in solution, reflecting surfaces…

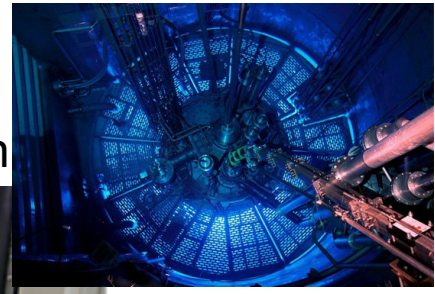
- Monitors - may probe the state of the neutron beam and store histograms / event lists



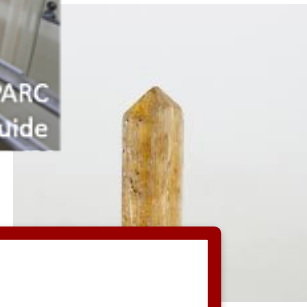
- Misc, obsolete
  - “Other stuff” and “Old stuff”

Component classes

- Sources - these define MC starting conditions / “inject” neutrons to our simulation



- Optics - used to tailor properties of the neutron beam
  - Examples are mirrors, guides, choppers, collimators, slits, …

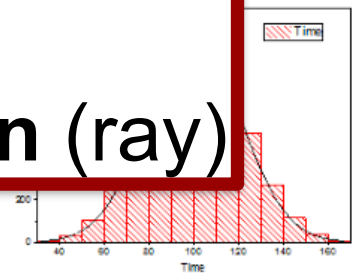


- Samples - “matter” of some form
  - Powders, single crystals, liquids, micelles in solution, reflecting surfaces
- Monitors - may probe

Common to all components:

They set, manipulate/interact with

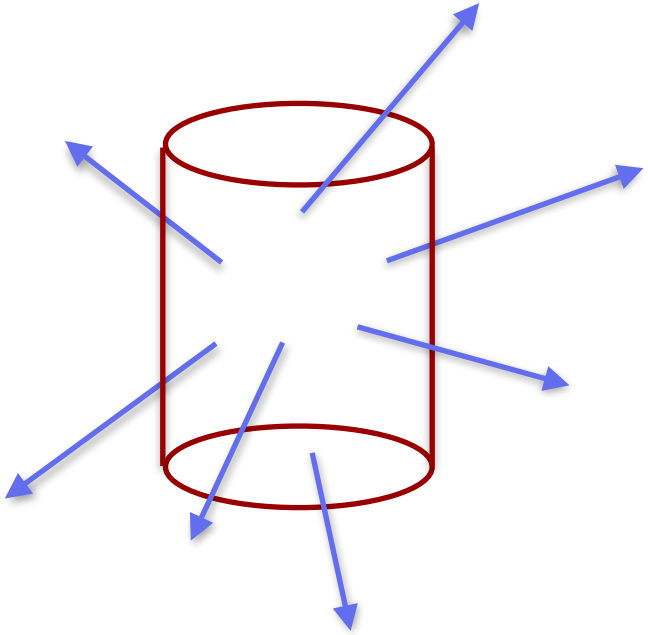
or measure the **state of the neutron** (ray)



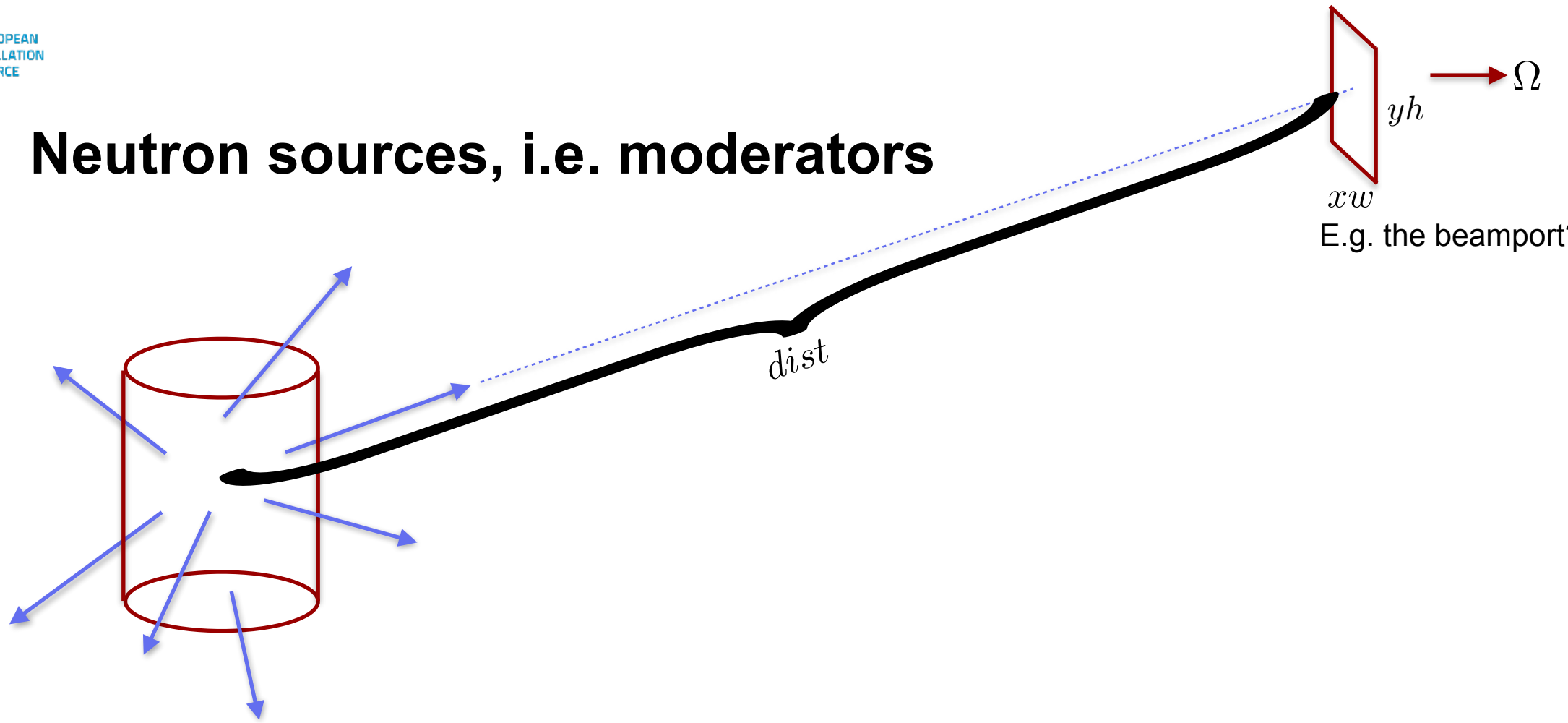
- Misc, obsolete
  - “Other stuff” and “Old stuff”

Neutron sources, i.e. moderators

- To first order emit uniformly into 4π steradian



Neutron sources, i.e. moderators

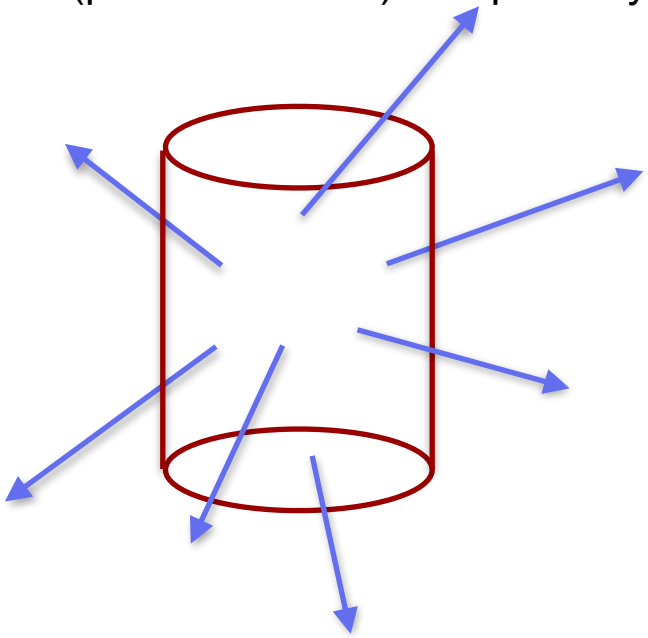


E.g. the beamport?

- Generally we are intersted in the input to a single instrument, characterised by a certain solid angle Ω, often corresponding to a rectangle xwx yh at a distance $dist$ from the source

Neutron sources, i.e. moderators

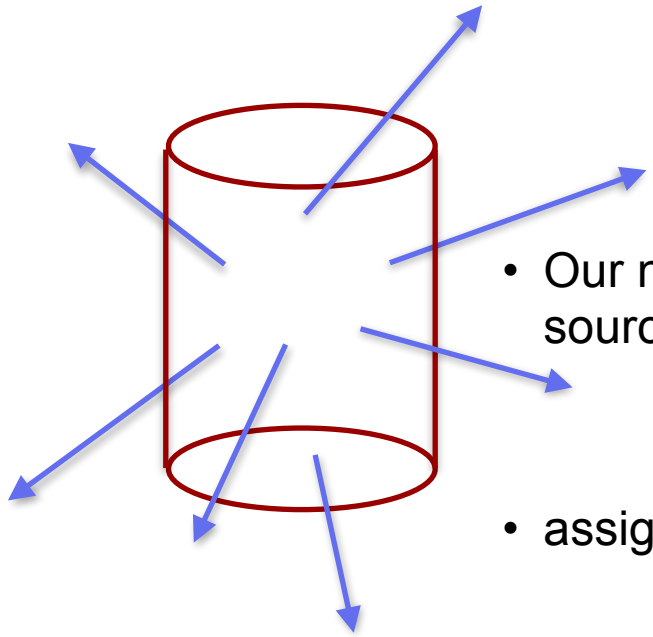
- The emmission intensity into our chosen solid angle Ω can be a function of wavelength, time (pulsed sources) and possibly point of origin on the source surface

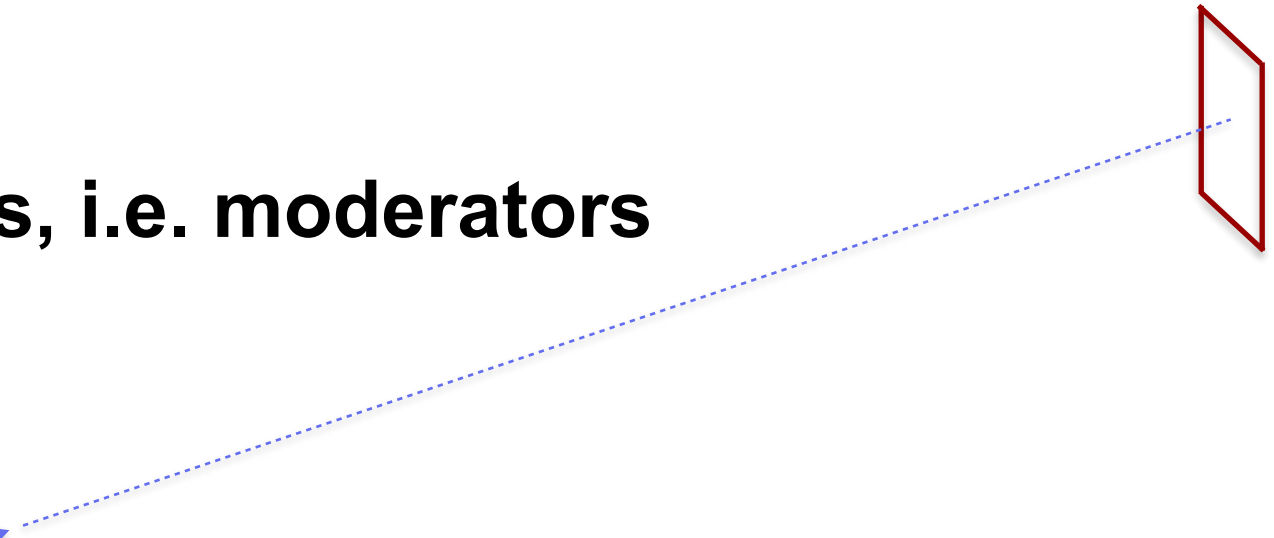


$$I(\lambda) \quad \Omega \quad [n/s/str]$$
$$I(\lambda, t) \quad \Omega \quad [n/s/str]$$
$$I(\lambda, t, \vec{r}) \quad \Omega \quad [n/s/str]$$

- The emission of particles into the solid angle Ω is in fact an integration and leads to a simulated "intensity" of $I_\Omega \ [n/s]$.
- In McStas, that integrated intensity is partitioned over a given set of particle *rays* referred to as **ncount**, -**n** or **--ncount**
- The default **ncount** is 1e6 rays

Neutron sources, i.e. moderators





- Our neutron rays are emitted randomly, sampling Ω and all variables of the source “spectrum”, i.e. wavelength, time and area

$$I_\Omega(\lambda, t, \vec{r}) \ [n/s]$$

- assigning neutron weights p such that

$$\sum_{j=1}^{\mathrm{ncount}} p_j = \int_{d\lambda, dt, d\vec{r}} I_\Omega(\lambda, t, \vec{r})$$

Neutron rays in McStas - what are they?

- Defining the neutron starting conditions imply setting:
  - The **starting point** on the surface, i.e. $\vec{r}$ (in the code variables `x,y,z`)
  - The **direction** into Ω and our λ/E_{kin} (in the code variables `vx,vy,vz`)
  - The **starting time** (in the code the variable `t`)
  - The initial **intensity** / weight of the neutron ray (in the code the variable `p`)
  - If needed the initial **polarisation** (in the code the variables `sx,sy,sz`)

Neutron **ray** in McStas:	
Location	`x,y,z`
Velocity	`vx,vy,vz`
Time	`t`
Polarisation.	`sx,sy,sz`
Intensity	`p`

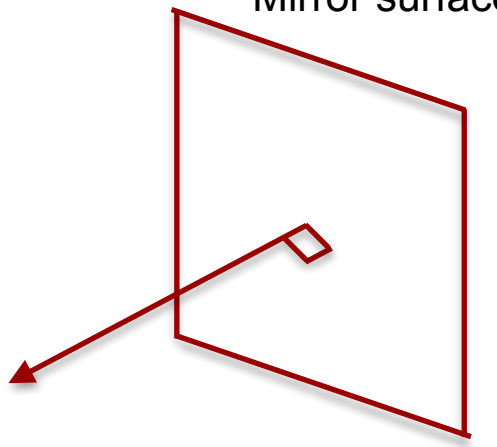
Neutron (ray)-matter interaction 1: reflecting surface

- 1 starting situation

Mirror surface

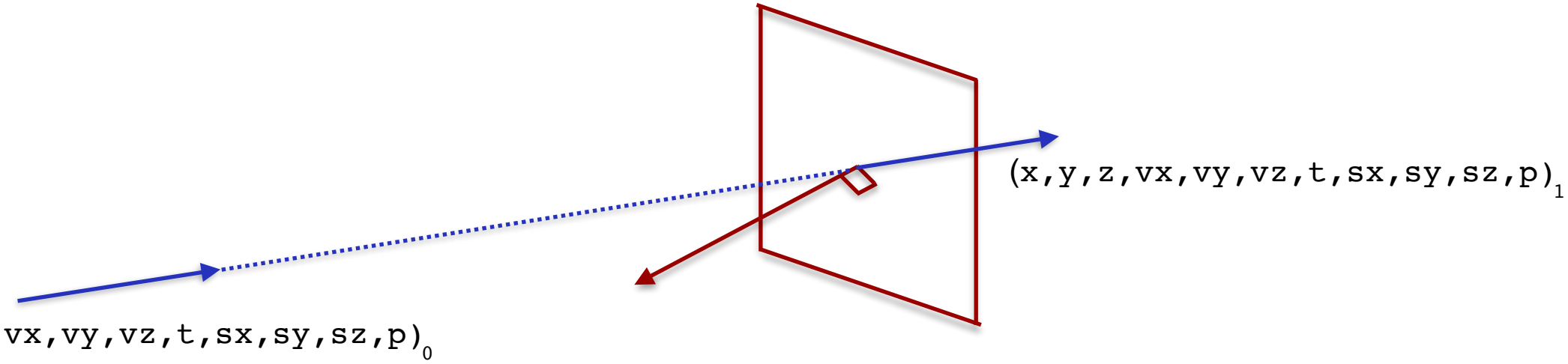
Neutron ray

$(x,y,z,vx,vy,vz,t,sx,sy,sz,p)_0$



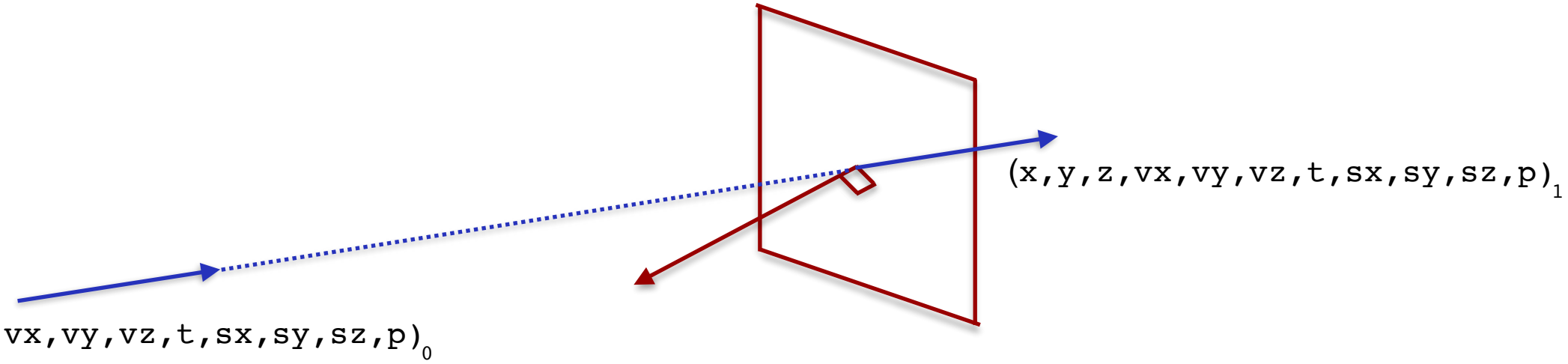
Neutron (ray)-matter interaction 1: reflecting surface

- 2. Propagate to the mirror surface



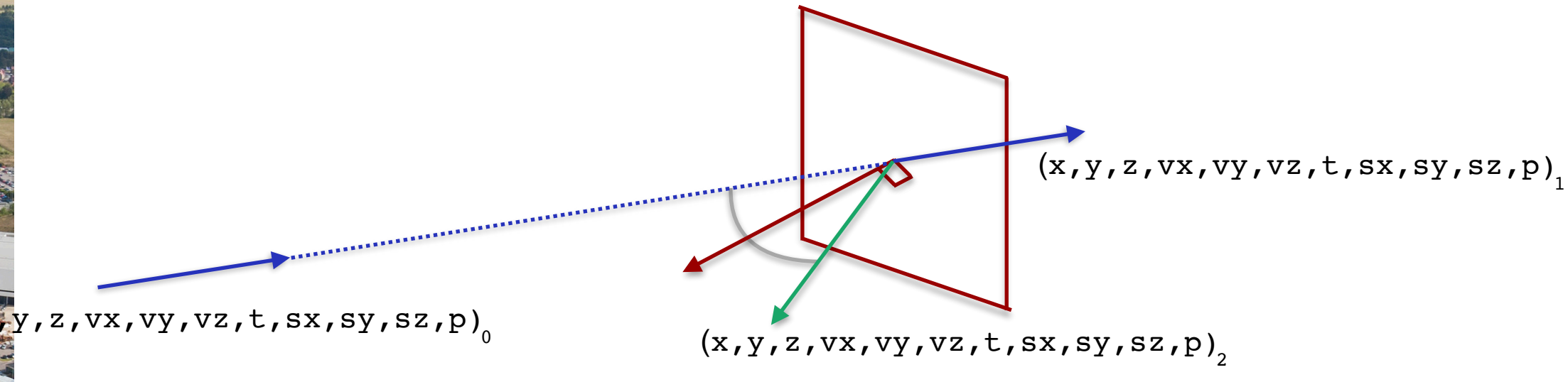
Neutron (ray)-matter interaction 1: reflecting surface

- 3. Checks (are we on surface, what is probability of reflection etc.)



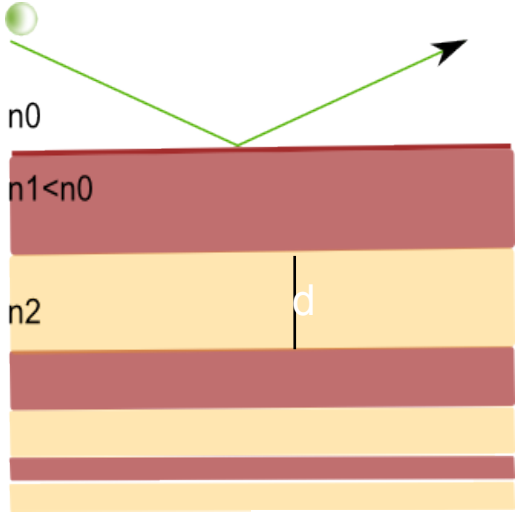
Neutron (ray)-matter interaction 1: reflecting surface

- 4. Reflect



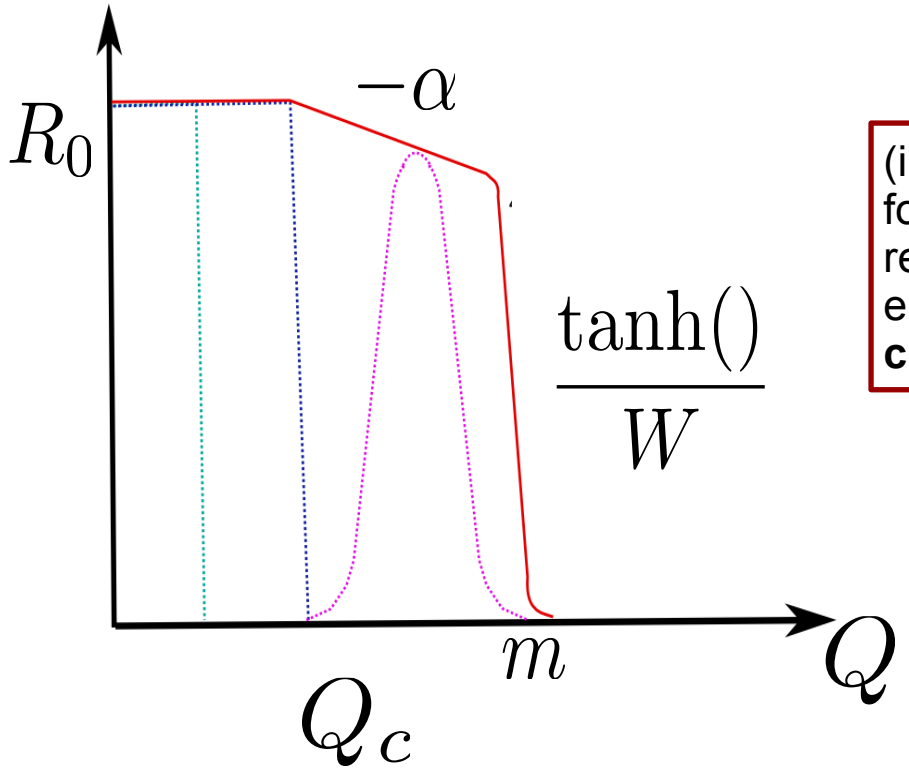
Weight of final ray is adjusted according to reflectivity, see next slide

Parametrisation of reflectivity on mirrors etc.



$$R_0 \cdot \left(1 - \frac{\tanh\left(Q - mQ_c\right)}{W}\right) \cdot \left(1 - \alpha(Q - Q_c)\right)$$

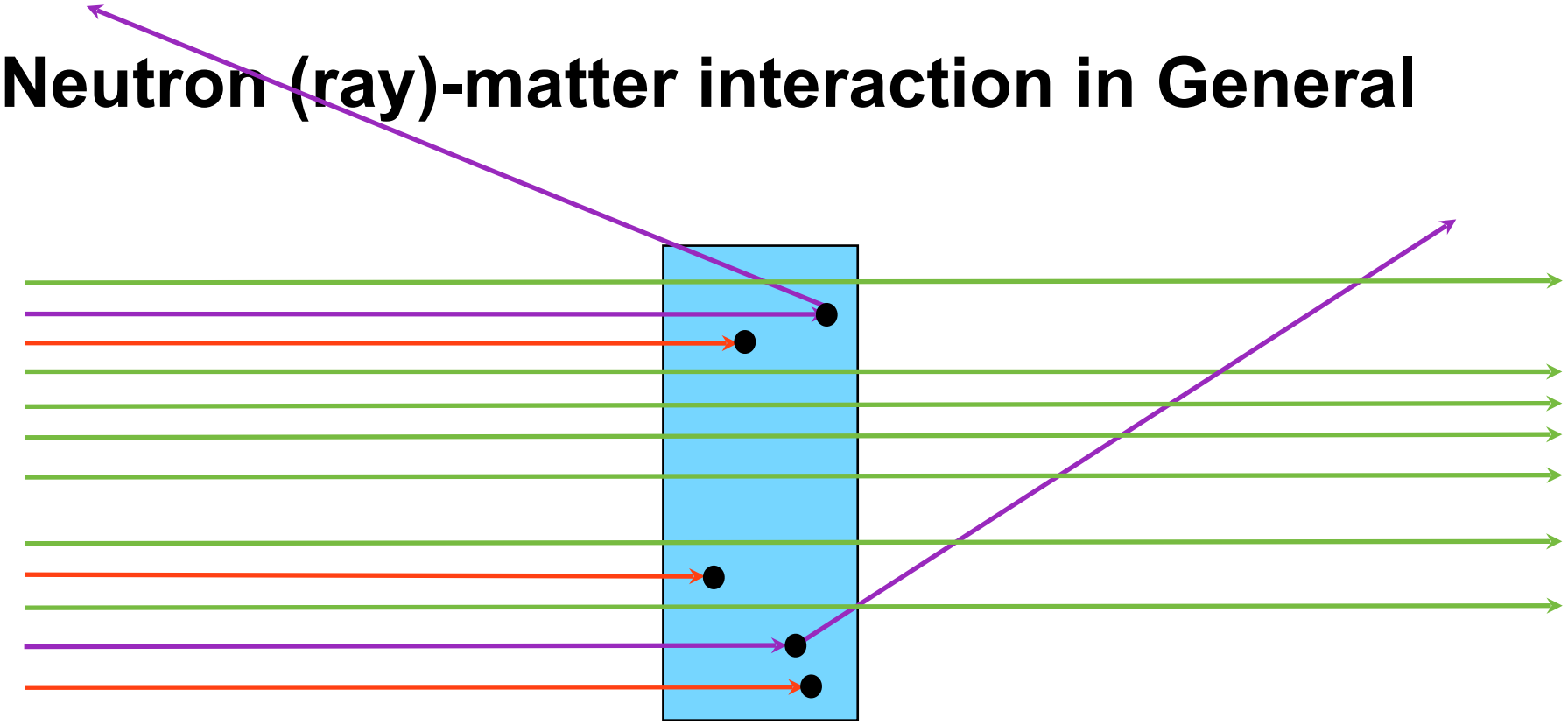
$$V = \frac{2\pi\hbar^2}{m} bN \qquad \sin\theta < \sqrt{\frac{mV}{2\pi^2\hbar^2}}\lambda$$



(i.e. Q is calculated for given neutron, reflectivity encoded in **changed *p* value**)

$$m = \frac{\theta_{mirror}}{\theta_{Ni}}$$

Neutron (ray)-matter interaction in General



absorbed, transmitted, or scattered

For a **non-thin** sample the probabilities for absorption, transmission or scattering are given by

$$p_A = (1 - e^{-\Sigma_T t})(\Sigma_A / \Sigma_T)$$

$$p_S = (1 - e^{-\Sigma_T t})(\Sigma_S / \Sigma_T)$$

$$p_T = 1 - p_S - p_A = e^{-\Sigma_T t}$$

t = sample thickness

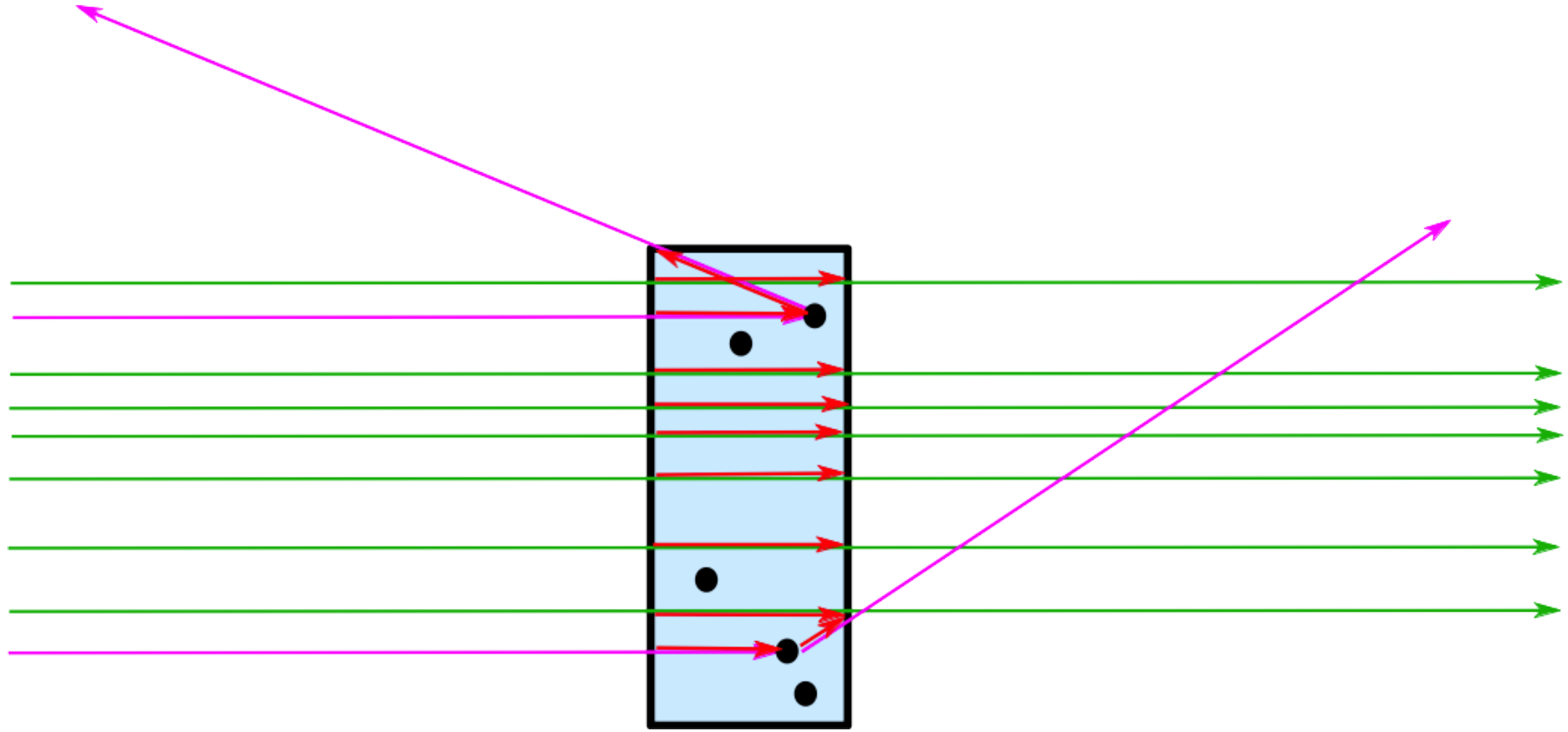
$$\Sigma_* = \rho \sigma_*$$

macroscopic cross section [cm^{-1}]

number density [$atoms/cm^3$]

microscopic cross section [barn/atom]
1 barn = $10^{-24} cm^2$

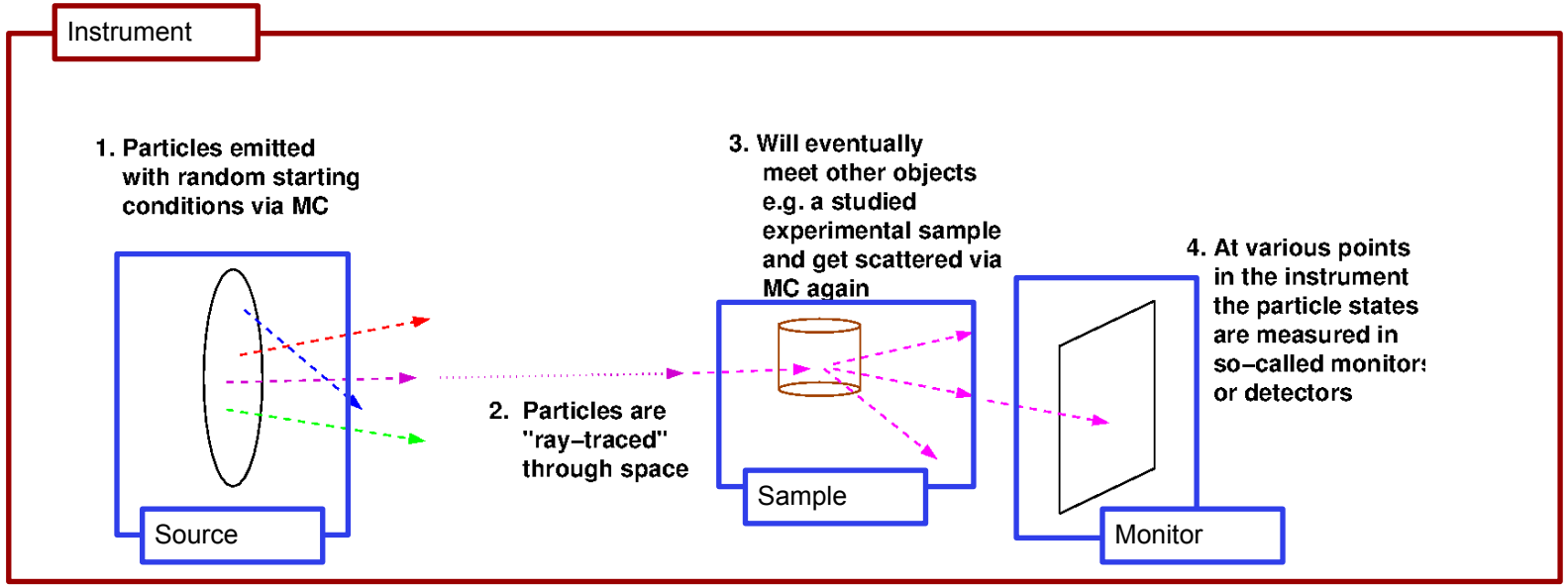
Samples/Matter interaction in General in McStas



transmitted+absorption, or scattered+absorption

Transport of weight through the instrument…

In a given component, the neutron intensity is adjusted by a multiplicative factor (probability)



p_0 p_j p_n

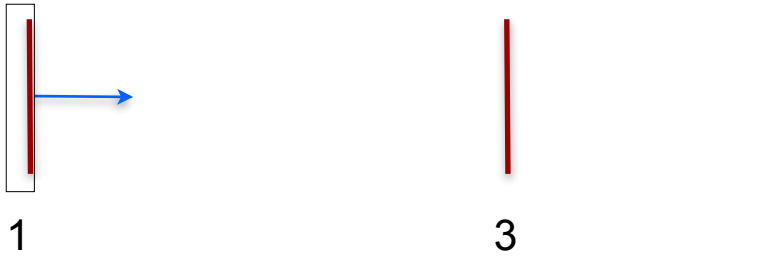
$$p_j = w_j p_{j-1}$$

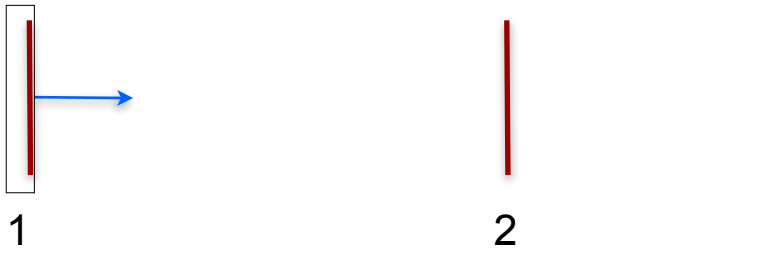
$$p_j = p_0 \prod_{k=1}^{j} w_k$$

The weight multiplier of the j'th component, w_j, is calculated by the probability rule $f_{\mathrm{MC,b}} w_j = P_{\mathrm{b}}$ where Pb is the physical probability for the event "b", and $f_{MC,b}$ is the probability that the Monte Carlo simulation selects this event.

In case of "branching", i.e. multiple outcomes, it is clear that $\sum_b f_{\mathrm{MC,b}} = 1$

To first order, McStas is linear and follows sequence of components in your file…



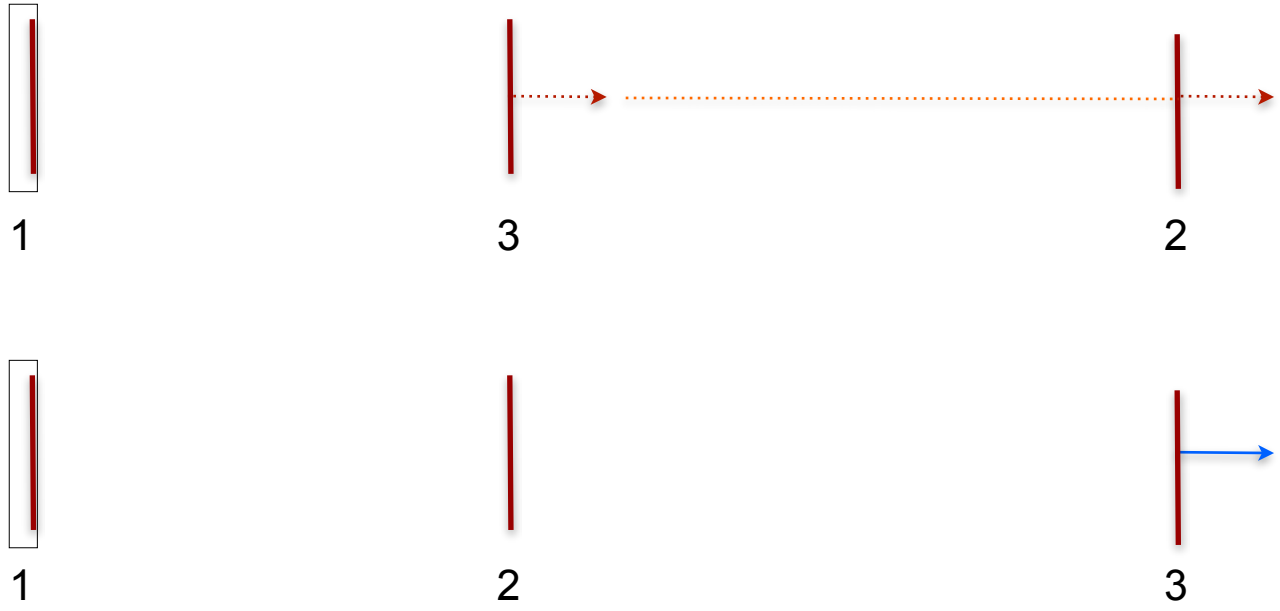


Starting at the source

To first order, McStas is linear and follows sequence of components in your file…

Moving to first comp in the list

To first order, McStas is linear and follows sequence of components in your file…



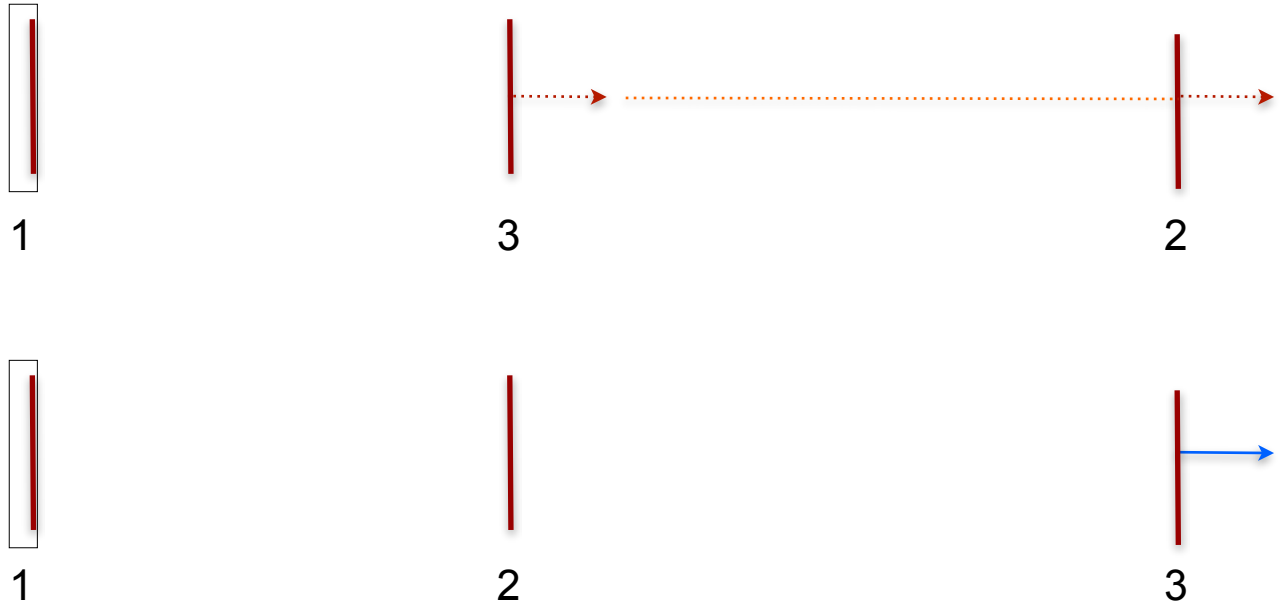
Moving to 3rd comp in list requires “moving back in time”.

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.

To first order, McStas is linear and follows sequence of components in your file…



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.

The order of components is important,

and in general overlaps should be avoided!

Instrument file

```
DEFINE INSTRUMENT My_Instrument(DIST=10)

/* Here comes the TRACE section, where the actual      */
/* instrument is defined as a sequence of components.  */
TRACE

/* The Arm() class component defines reference points and orientations  */
/* in 3D space.                                                         */
COMPONENT Origin = Arm()
  AT (0,0,0) ABSOLUTE


COMPONENT Source = Source_simple(
    radius = 0.1, dist = 10, xw = 0.1, yh = 0.1, E0 = 5, dE = 1)
  AT (0, 0, 0) RELATIVE Origin


COMPONENT Emon = E_monitor(
    filename = "Emon.dat", xmin = -0.1, xmax = 0.1, ymin = -0.1,
    ymax = 0.1, Emin = 0, Emax = 10)
  AT (0, 0, DIST) RELATIVE Origin


COMPONENT PSD = PSD_monitor(
    nx = 128, ny = 128, filename = "PSD.dat", xmin = -0.1,
    xmax = 0.1, ymin = -0.1, ymax = 0.1)
  AT (0, 0, 1e-10) RELATIVE Emon

/* The END token marks the instrument definition end */
END
```

Written by you!

Component file


```
/*******************************************************************************
*
* Mcstas, neutron ray-tracing package
*         Copyright 1997-2002, All rights reserved
*         Risoe National Laboratory, Roskilde, Denmark
*         Institut Laue Langevin, Grenoble, France
*
* Component: Source_flat
*
* %I
* Written by: Kim Lefmann
* Date: October 30, 1997
* Modified by: KL, October 4, 2001
* Modified by: Emmanuel Farhi, October 30, 2001. Serious bug corrected.
* Version: $Revision: 1.22 $
* Origin: Risoe
* Release: McStas 1.6
*
* A circular neutron source with flat energy spectrum and arbitrary flux
*
* %D
* The routine is a circular neutron source, which aims at a square target
* centered at the beam (in order to improve MC-acceptance rate).  The angular
* divergence is then given by the dimensions of the target.
* The neutron energy is uniformly distributed between E0-dE and E0+dE.
*
* Example: Source_flat(radius=0.1, dist=2, xw=.1, yh=.1, E0=14, dE=2)
*
* %P
* radius: (m)   Radius of circle in (x,y,0) plane where neutrons
*               are generated.
* dist:   (m)   Distance to target along z axis.
* xw:     (m)   Width(x) of target
* yh:     (m)   Height(y) of target
* E0:     (meV) Mean energy of neutrons.
* dE:     (meV) Energy spread of neutrons.
* Lambda0 (AA)  Mean wavelength of neutrons.
* dLambda (AA)  Wavelength spread of neutrons.
* flux    (1/(s*cm**2*st)) Energy integrated flux
*
* %E
*******************************************************************************/

DEFINE COMPONENT Source_simple
DEFINITION PARAMETERS ()
SETTING PARAMETERS (radius, dist, xw, yh, E0=0, dE=0, Lambda0=0, dLambda=0, flux=1)
OUTPUT PARAMETERS ()
STATE PARAMETERS (x,y,z,vx,vy,vz,t,s1,s2,p)
DECLARE
%{
  double pmul, pdir;
%}
INITIALIZE
%{
  pmul=flux*PI*1e4*radius*radius/mcget_ncount();
%}
```

```
TRACE
%{
 double chi,E,Lambda,v,r, xf, yf, rf, dx, dy;

 t=0;
 z=0;

 chi=2*PI*rand01();                          /* Choose point on source */
 r=sqrt(rand01())*radius;                    /* with uniform distribution. */
 x=r*cos(chi);
 y=r*sin(chi);

 randvec_target_rect(&xf, &yf, &rf, &pdir,
        0, 0, dist, xw, yh, ROT_A_CURRENT_COMP);

 dx = xf-x;
 dy = yf-y;
 rf = sqrt(dx*dx+dy*dy+dist*dist);

 p = pdir*pmul;

 if(Lambda0==0) {
   E=E0+dE*randpm1();              /*  Choose from uniform distribution */
   v=sqrt(E)*SE2V;
 } else {
   Lambda=Lambda0+dLambda*randpm1();
   v = K2V*(2*PI/Lambda);
 }

 vz=v*dist/rf;
 vy=v*dy/rf;
 vx=v*dx/rf;
%}

MCDISPLAY
%{
  magnify("xy");
  circle("xy",0,0,0,radius);
%}

END
```

Written by developers and possibly you!

Generated c-code

```
/* Automatically generated file. Do not edit.
 * Format:     ANSI C source code
 * Creator:    McStas <http://neutron.risoe.dk>
 * Instrument: My_Instrument.instr (My_Instrument)
 * Date:       Sat Apr  9 15:27:56 2005
 */

/* THOUSANDS of lines removed here.... */

  /* TRACE Component Source. */
  SIG_MESSAGE("Source (Trace)");
  mcDEBUG_COMP("Source")
  mccoordschange(mcposrSource, mcrotrSource,
    &mcnlx, &mcnly, &mcnlz,
    &mcnlvx, &mcnlvy, &mcnlvz,
    &mcnlt, &mcnlsx, &mcnlsy);
  mcDEBUG_STATE(mcnlx, mcnly, mcnlz, mcnlvx, mcnlvy, mcnlvz,mcnlt,mcnlsx,mcnlsy, mcnlp)
#define x mcnlx
#define y mcnly
#define z mcnlz
#define vx mcnlvx
#define vy mcnlvy
#define vz mcnlvz
#define t mcnlt
#define s1 mcnlsx
#define s2 mcnlsy
#define p mcnlp
  STORE_NEUTRON(2,mcnlx, mcnly, mcnlz, mcnlvx,mcnlvy,mcnlvz,mcnlt,mcnlsx,mcnlsy, mcnlsz, mcnlp);
  mcScattered=0;
  mcNCounter[2]++;
#define mccompcurname Source
#define mccompcurindex 2
{   /* Declarations of SETTING parameters. */
MCNUM radius = mccSource_radius;
MCNUM dist = mccSource_dist;
MCNUM xw = mccSource_xw;
MCNUM yh = mccSource_yh;
MCNUM E0 = mccSource_E0;
MCNUM dE = mccSource_dE;
MCNUM Lambda0 = mccSource_Lambda0;
MCNUM dLambda = mccSource_dLambda;
MCNUM flux = mccSource_flux;
#line 58 "Source_simple.comp"
{
 double chi,E,Lambda,v,r, xf, yf, rf, dx, dy;

 t=0;
 z=0;

 chi=2*PI*rand01();                         /* Choose point on source */
 r=sqrt(rand01())*radius;                   /* with uniform distribution. */
 x=r*cos(chi);
 y=r*sin(chi);

 randvec_target_rect(&xf, &yf, &rf, &pdir,
        0, 0, dist, xw, yh, ROT_A_CURRENT_COMP);
```

Written by mcstas!

McStas is a (pre)compiler!

Input is .comp and .instr files + runtime functions for e.g. random numbers

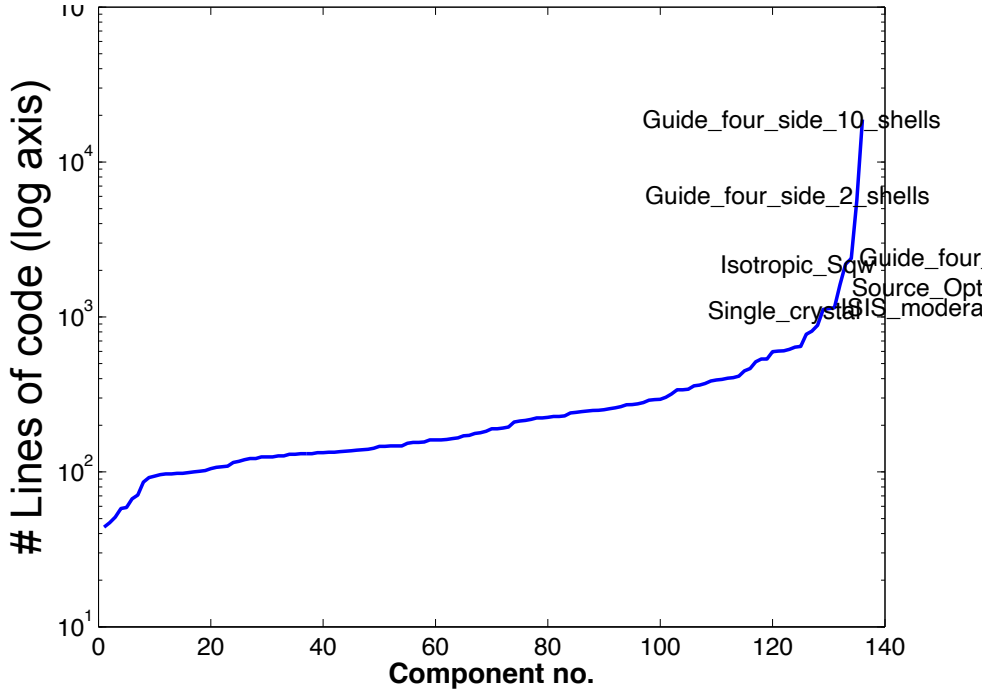
Output is a single c-file, which can be compiled using e.g. gcc.

Can take input arguments if needed.

Writing new comps or understanding existing is not that complex...

- Check our long list of components and look inside... Most of them are quite simple and short... Statistics:

Number of lines of code per component - 199 comps in total



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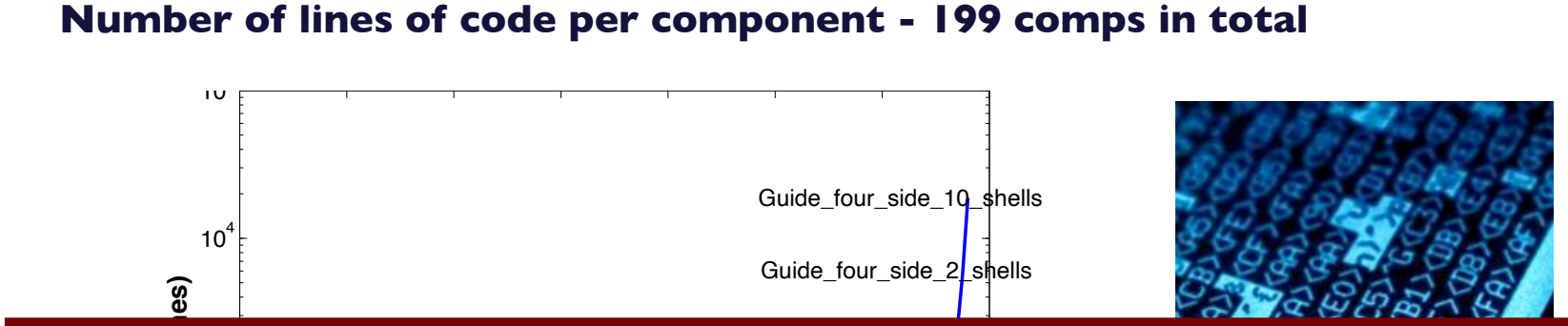
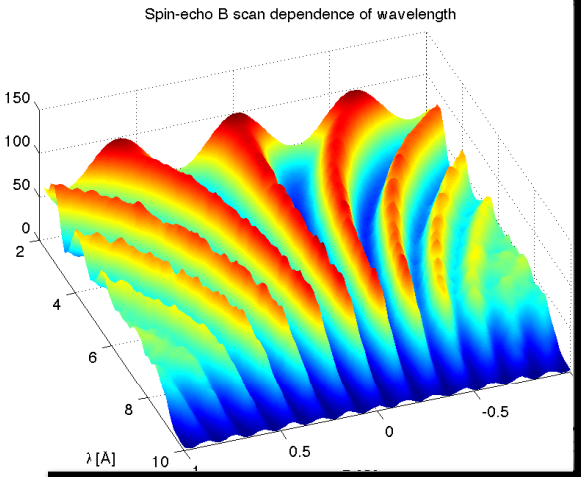
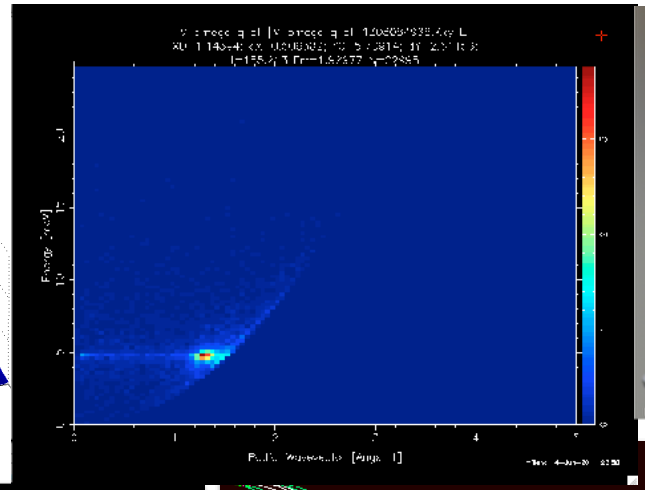
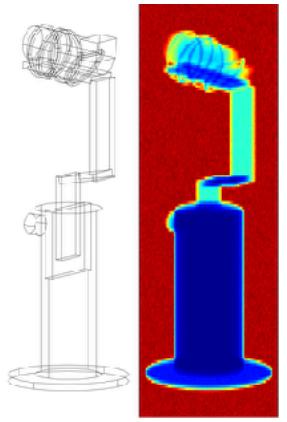


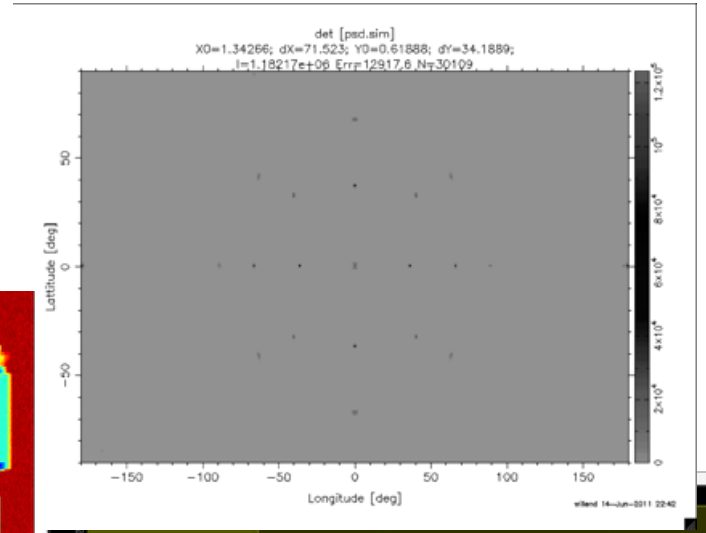
- Well-developed community support
  - –30-40% of existing and new additions are from users
  - –No direct refereeing of the code, but these requirements:
    - –At least one test-instrument
    - –Meaningful documentation headers (in-code docs)
  - –Contributions go in dedicated contrib/ section of library

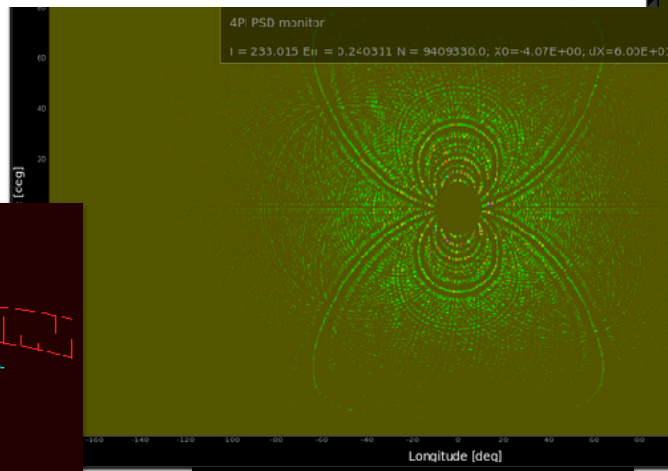
Example suite: ~140 instruments

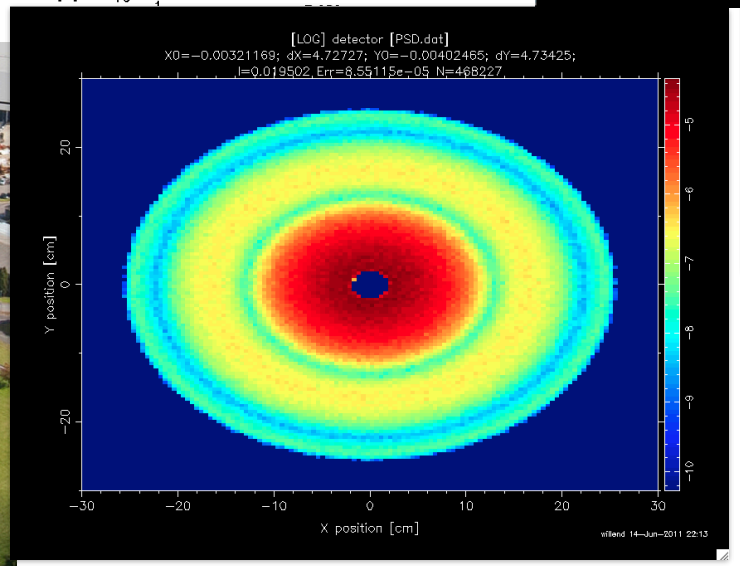


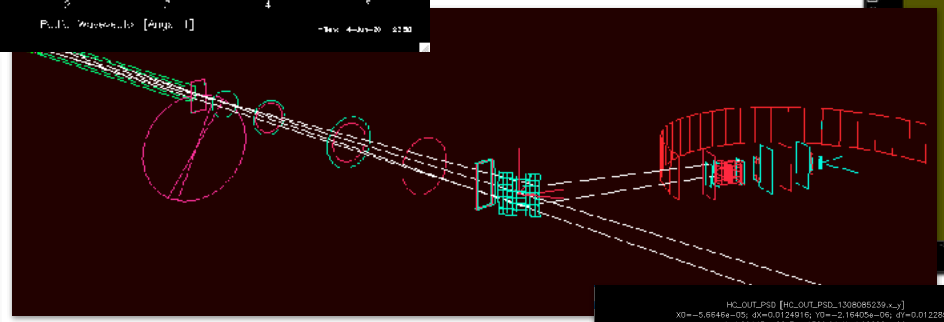


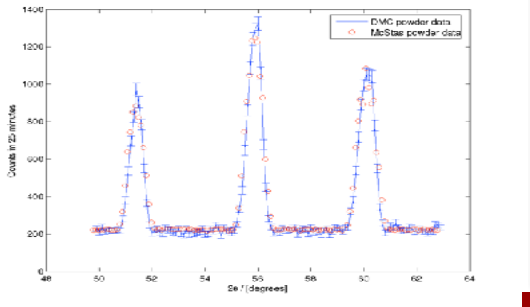


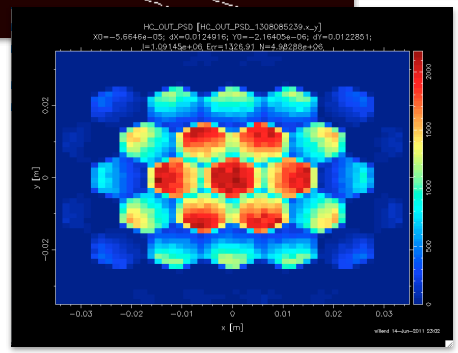


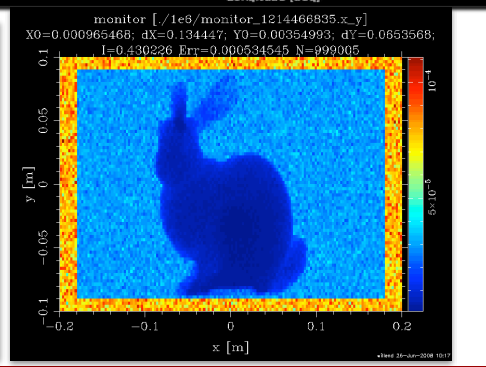


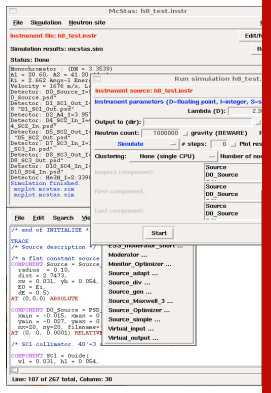


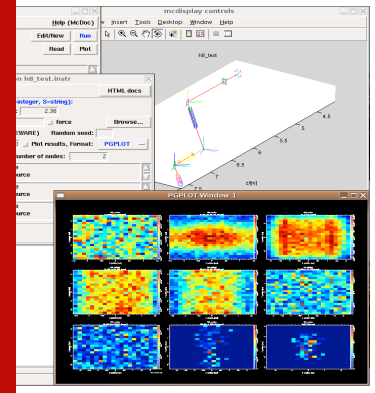












THIS IS NOT THE END

IT'S JUST THE BEGINNING