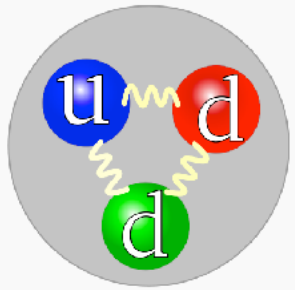
McStas Introduction and general concepts

Agenda

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

McStas: Neutrons, Monte Carlo & ray-tracing

Neutron



The quark structure of the neutron. (The color assignment of individual quarks is not important; what is important is that all three colors are present.)

Classification	Baryon
Composition	1 up quark, 2 down quarks
Statistics	Fermionic
Interactions	Gravity, Weak, Strong, Electromagnetic
Symbol	n^0, N^0
Antiparticle	Antineutron
Theorized	Ernest Rutherford[1][2] (1920)
Discovered	James Chadwick[1] (1932)
Mass	$1.674\,927\,351(74) \times 10^{-27}$ kg[3] 939.565 378(21) MeV/c^2[3] 1.008 664 916 00(43) u[3]
Mean lifetime	881.5(15) s (free)
Electric charge	0 e 0 C
Electric dipole moment	$<2.9 \times 10^{-26}$ e·cm
Electric polarizability	$1.16(15) \times 10^{-3}$ fm^3

$$\text{Life time:} \quad \tau_{1/2} = 890s$$
$$\text{Mass:} \quad m = 1.675 \times 10^{-27} kg$$
$$\text{Charge:} \quad Q = 0$$
$$\text{Spin:} \quad s = \hbar/2$$
$$\text{Magnetic moment:} \quad \mu/\mu_n = -1.913$$

$$E = \frac{1}{2}mv^2 = \frac{\hbar^2 k^2}{2m}, \qquad \lambda = 2\pi/k$$

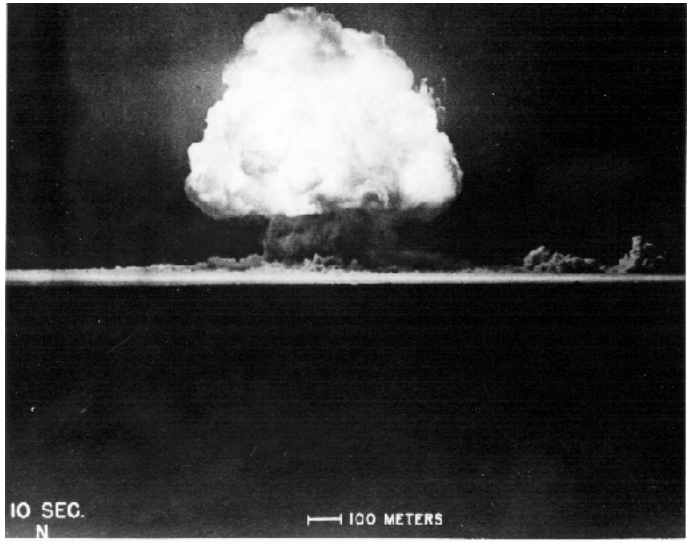
$$E = 81.81 \cdot \lambda^{-2} = 2.07 \cdot k^2 = 5.23 \cdot v^2$$

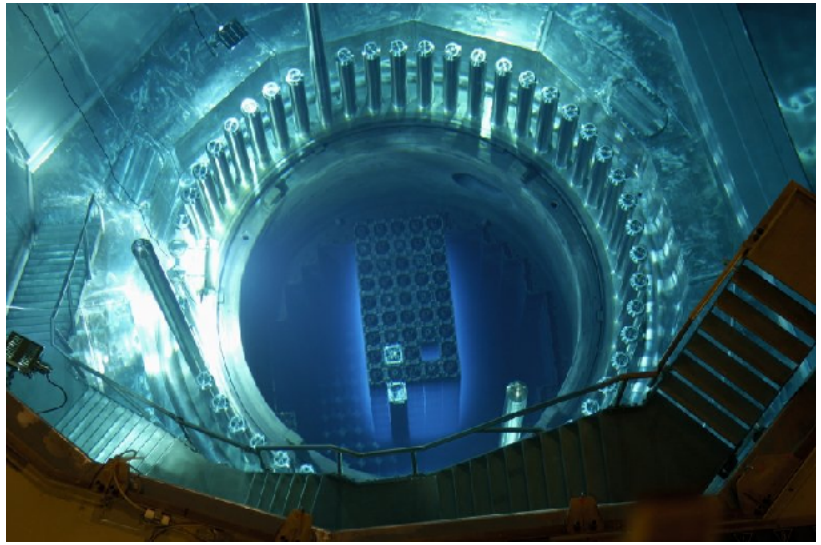
Subatomic particle discovered by Sir James Chadwick in 1932

	Energy	Wavelength	n-Wavevector	Velocity	Frequency
cold neutrons:	E = 1 meV	l = 9.0446 Å	k = 0.6947 1/Å	v = 437 m/s	v = 0.2418 THz
	E = 5 meV	l = 4.0449 Å	k = 1.5534 1/Å	v = 978 m/s	v = 1.2090 THz
thermal neutrons:	E = 25 meV	l = 1.8089 Å	k = 3.4734 1/Å	v = 2187 m/s	v = 6.045 THz
	E = 50 meV	l = 1.2791 Å	k = 4.9122 1/Å	v = 3093 m/s	v = 12.090 THz

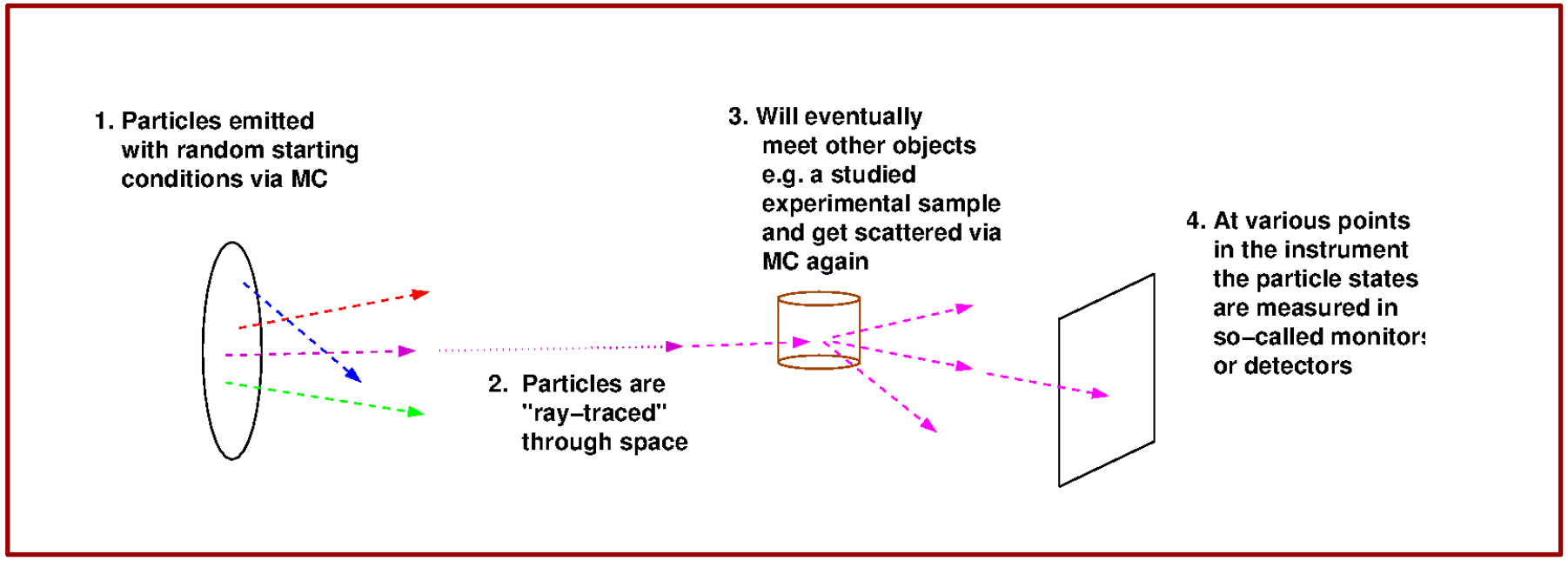
Monte Carlo techniques

- Los Alamos has since then developed and perfected many different monte carlo codes leading to what is today known as the codes MCNP5 and MCNPX
- State of the art is MCNP6 that features numerous (even exotic) particles
- MCNP was originally Monte Carlo Neutron Photon, later N-Particle
- Mainly used for high-energy particle descriptions in weapons, power reactors and routinely used for estimating dose rates and needed shielding
- Not much focus on crystalline / ordered material and coherent scattering of neutrons due to the focus on high energies

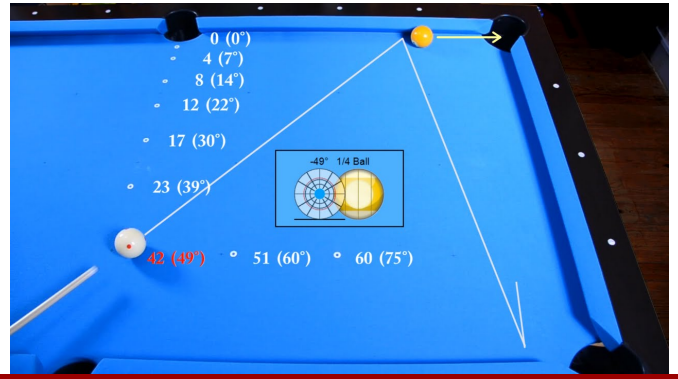




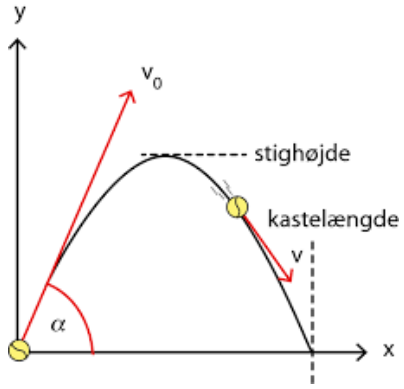
In the big picture, McStas is this…



- Classical Newtonian mechanics, i.e.



and



- (independent, particles though…)

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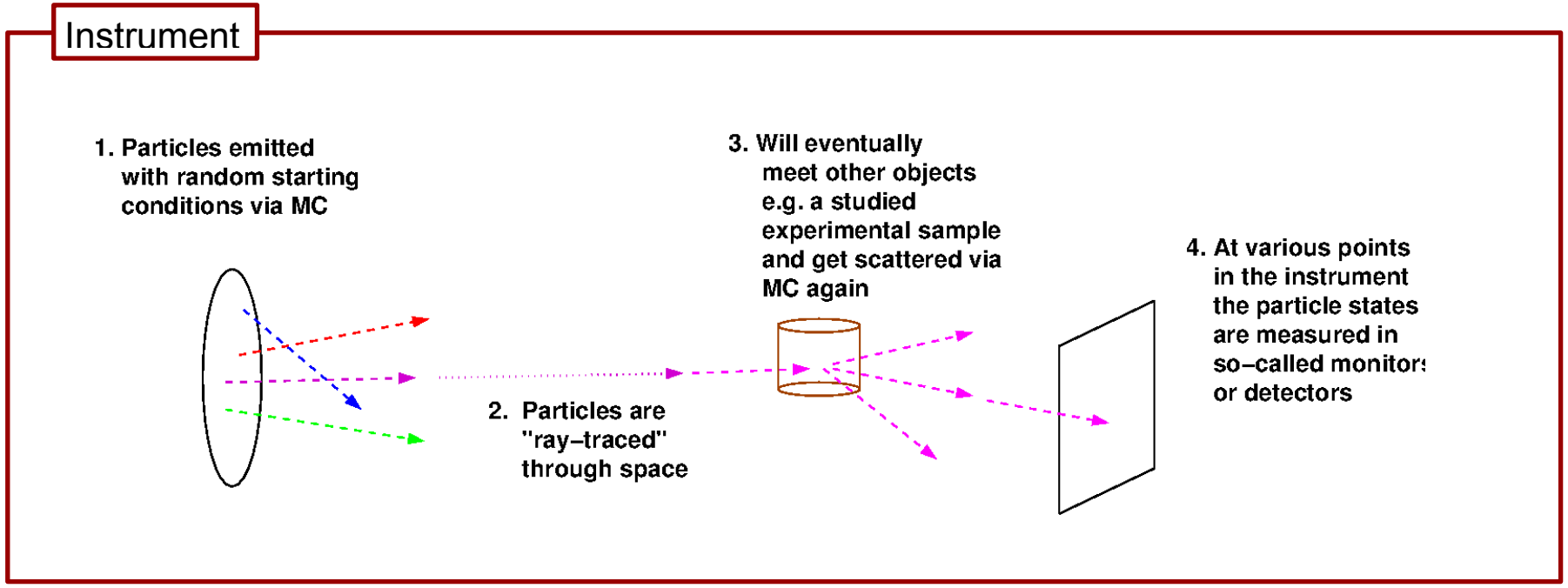
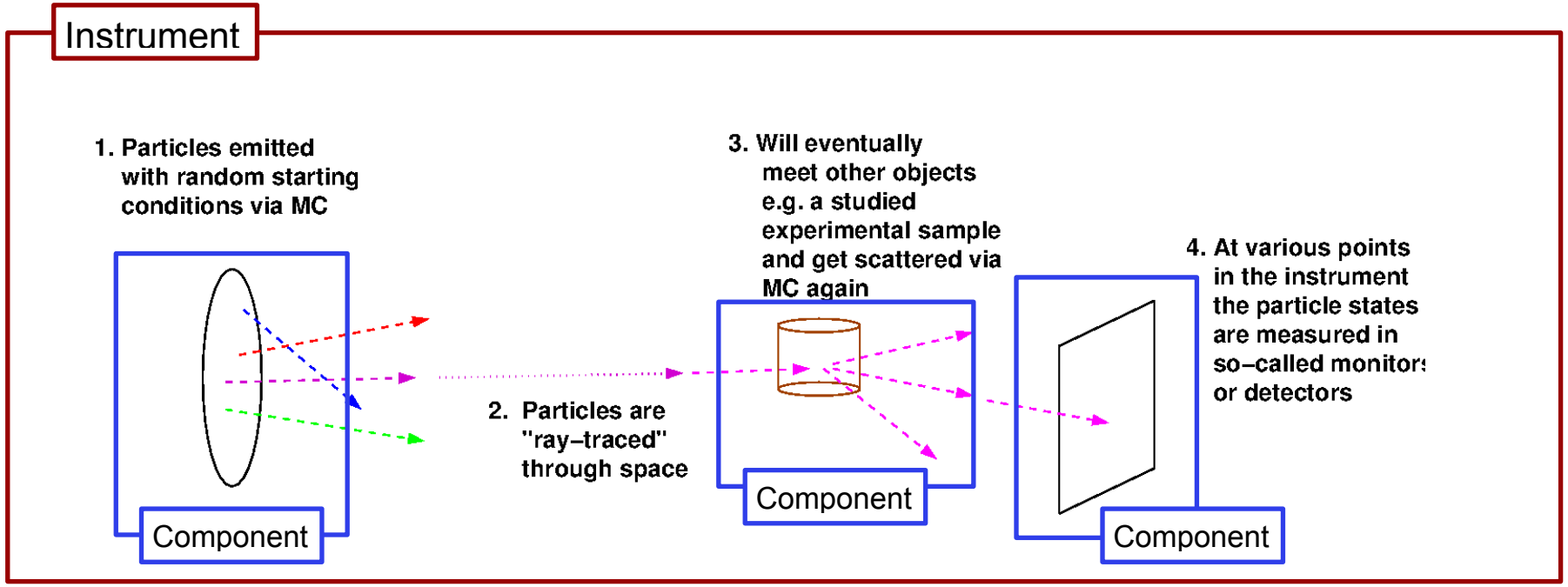


The instrument defines our “lab coordinate system”

In the big picture, McStas is this…



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The components define devices or features available in our instrument

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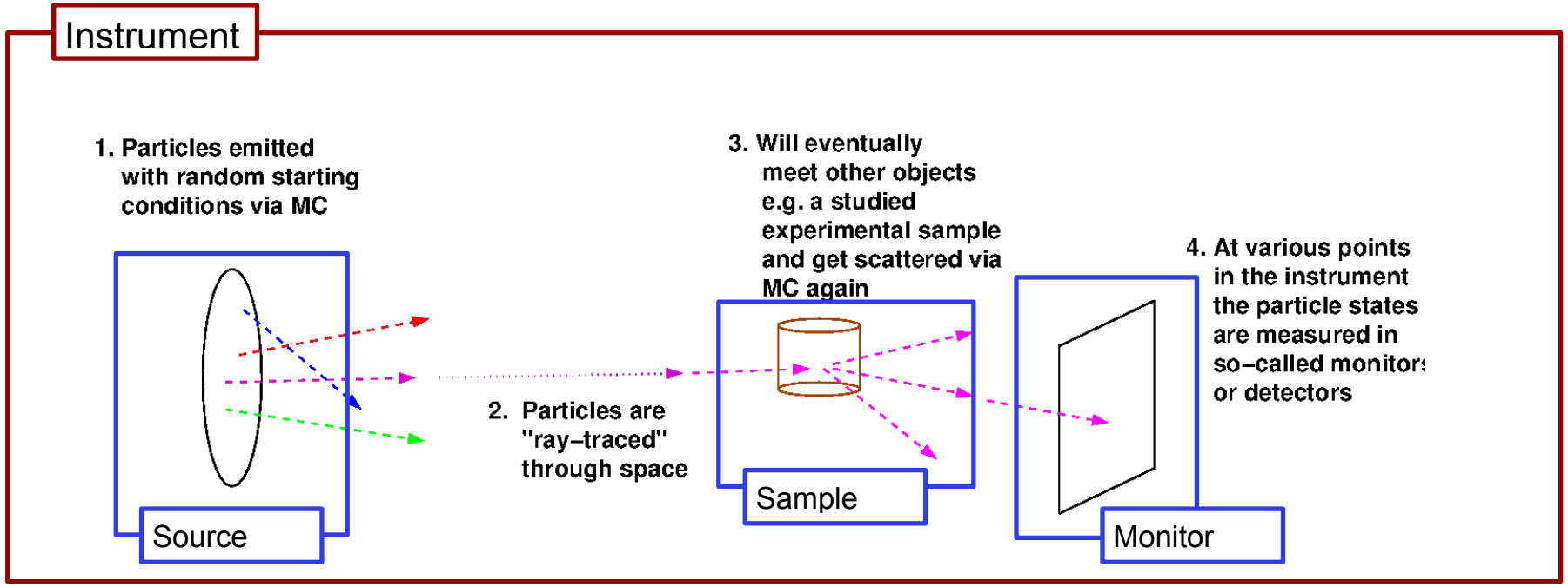

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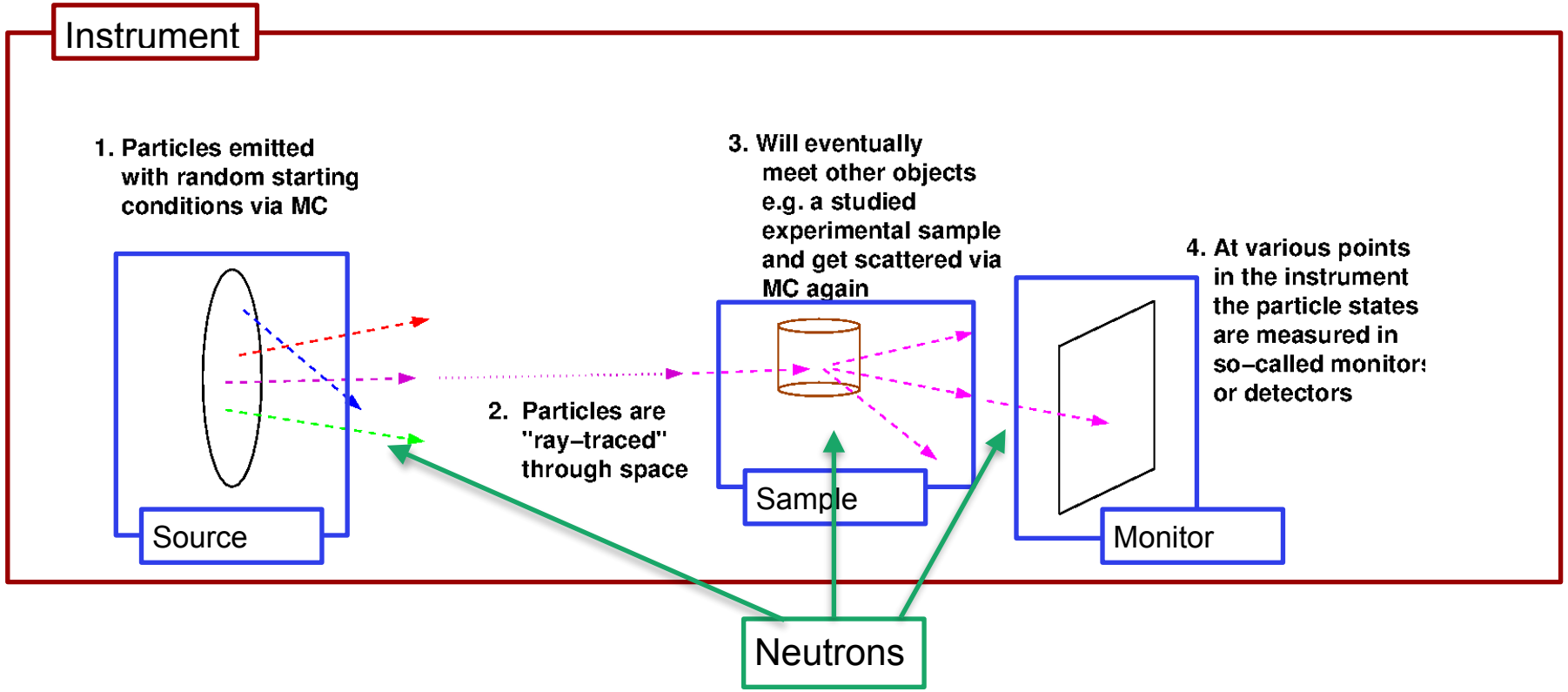

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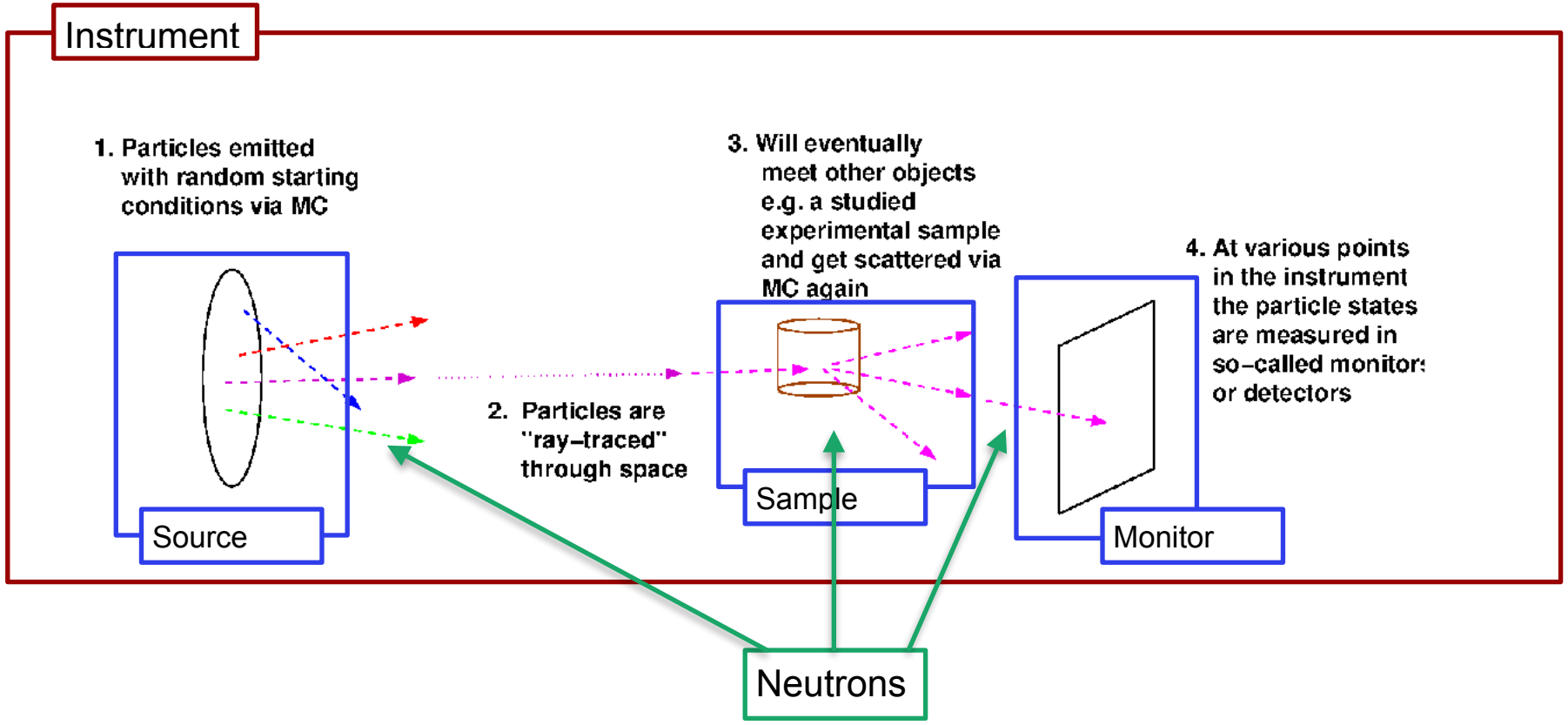
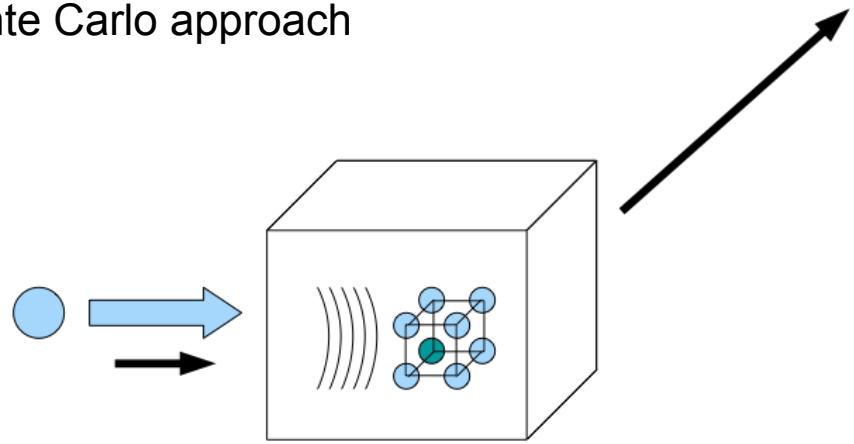
Neutron particles are passed on from one component to the next, changing state under way

McStas is a Monte Carlo ray-tracer



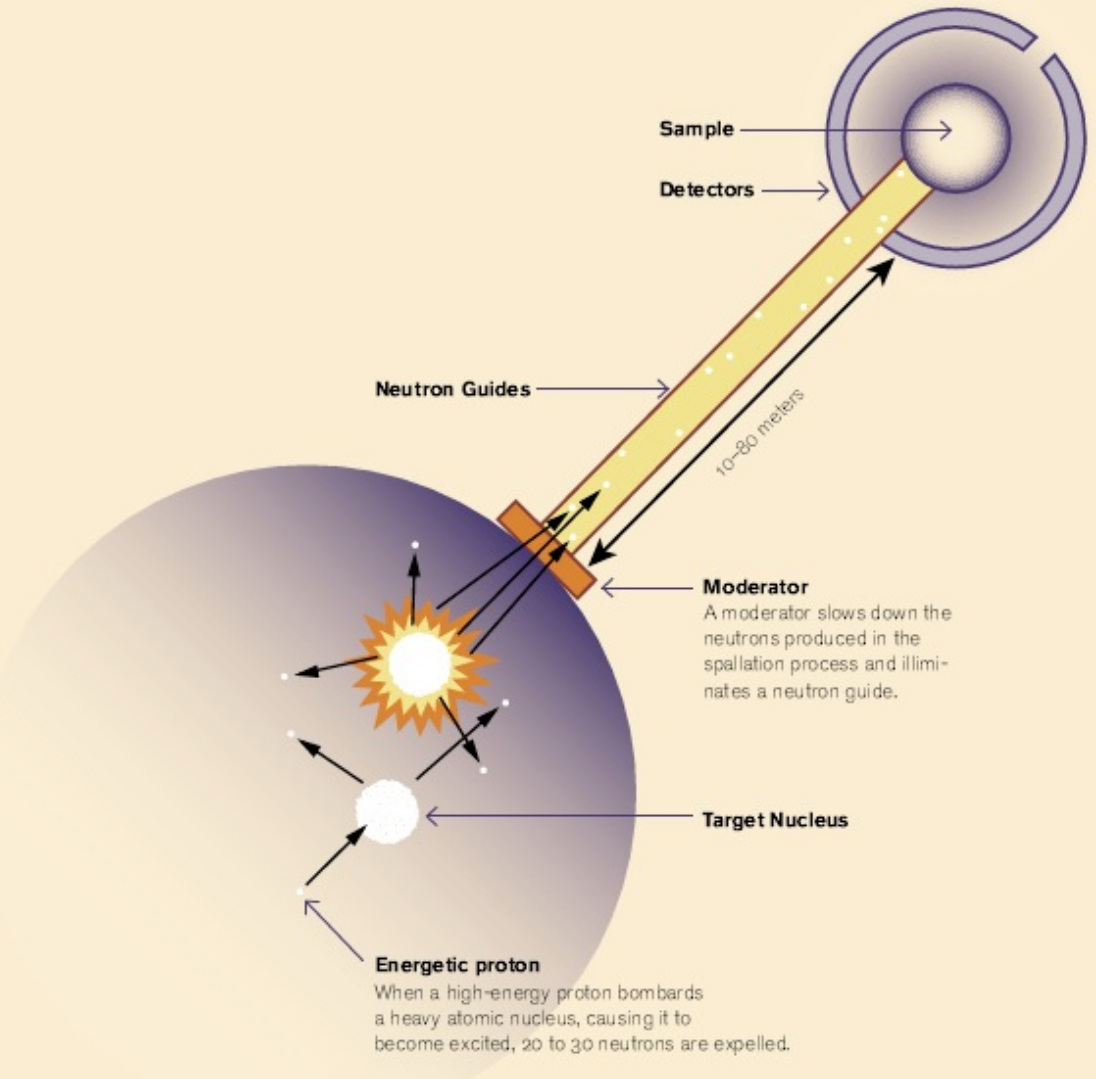
Elements of Monte-Carlo raytracing

- 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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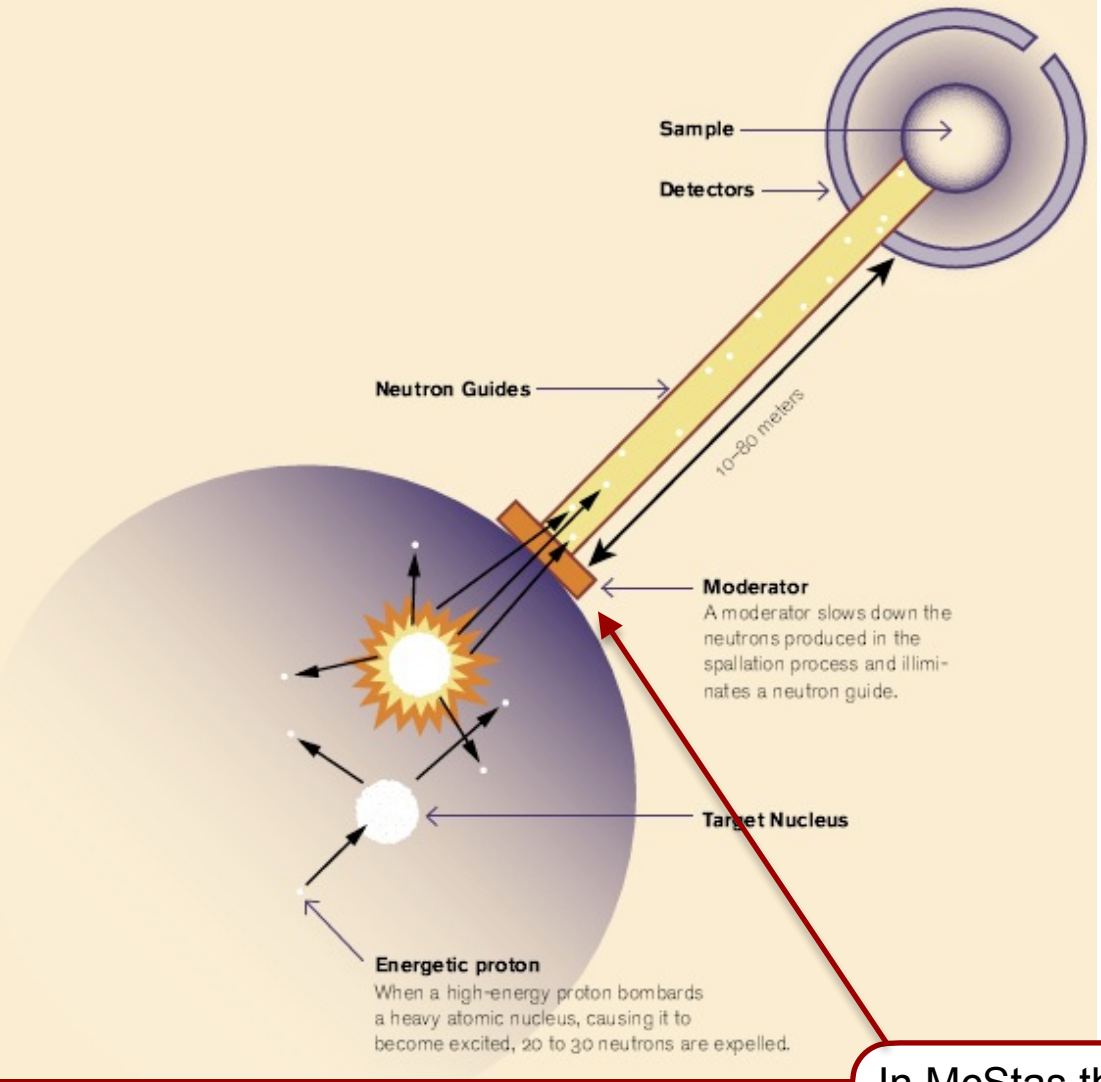
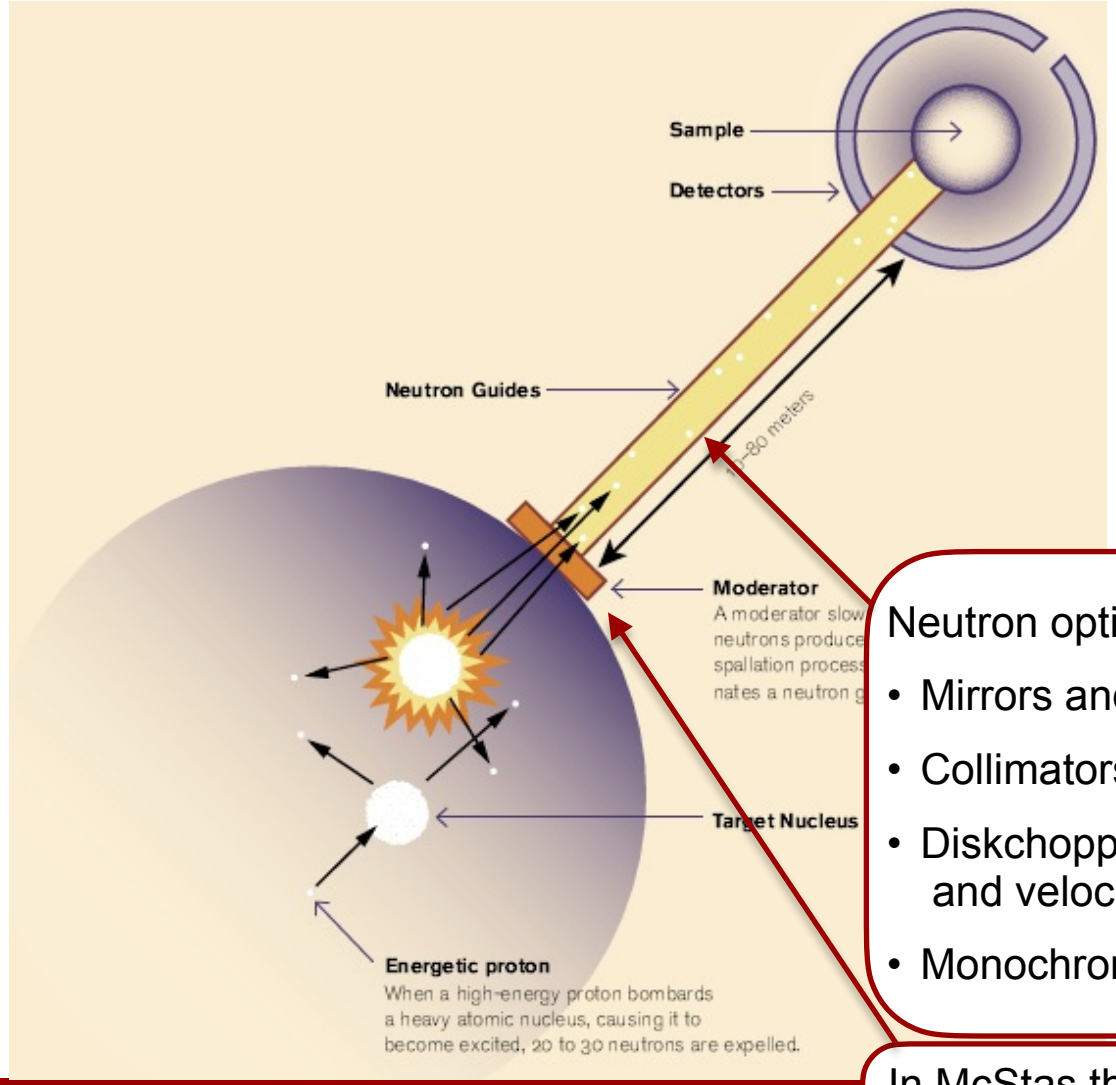


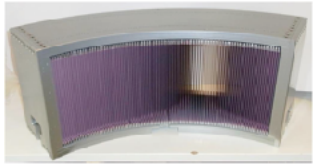
In McStas the moderator is the “source”

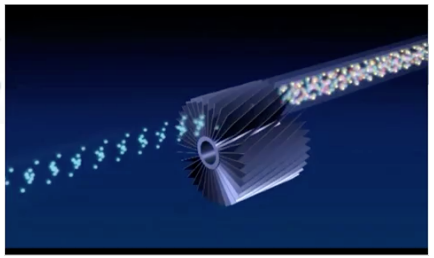
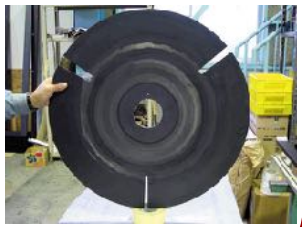
Components of neutron instruments



Neutron optics include things like:

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

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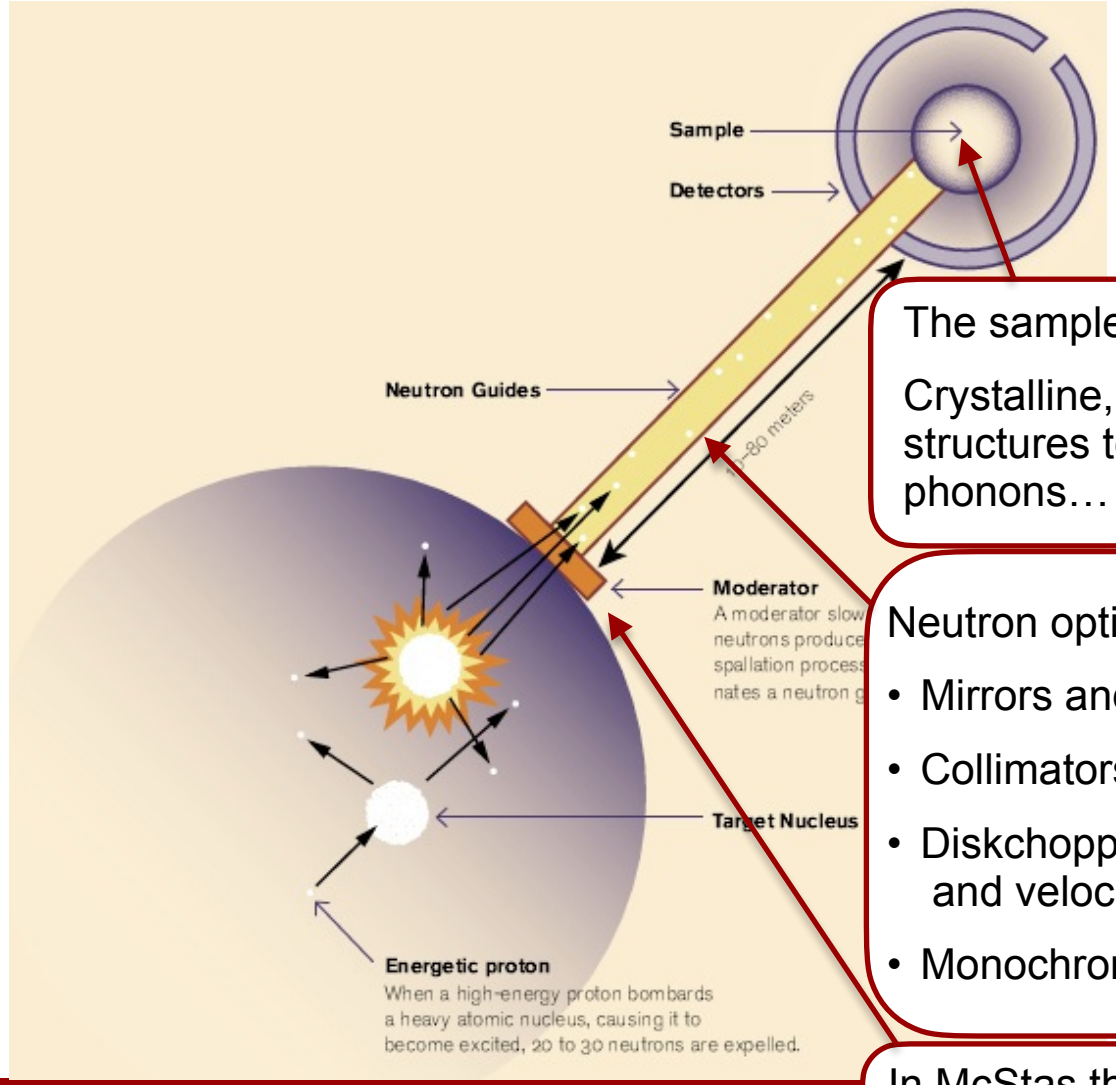
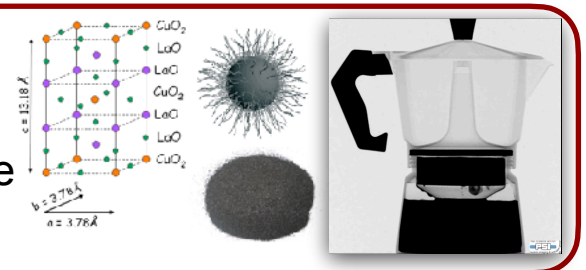


The sample:

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



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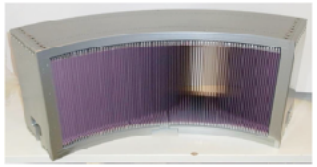

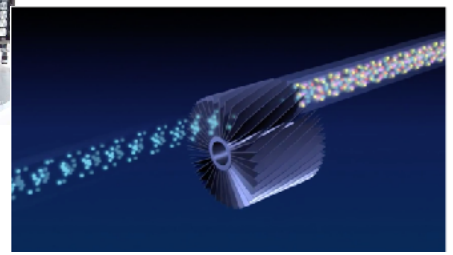
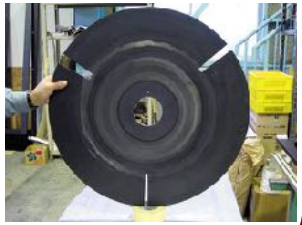

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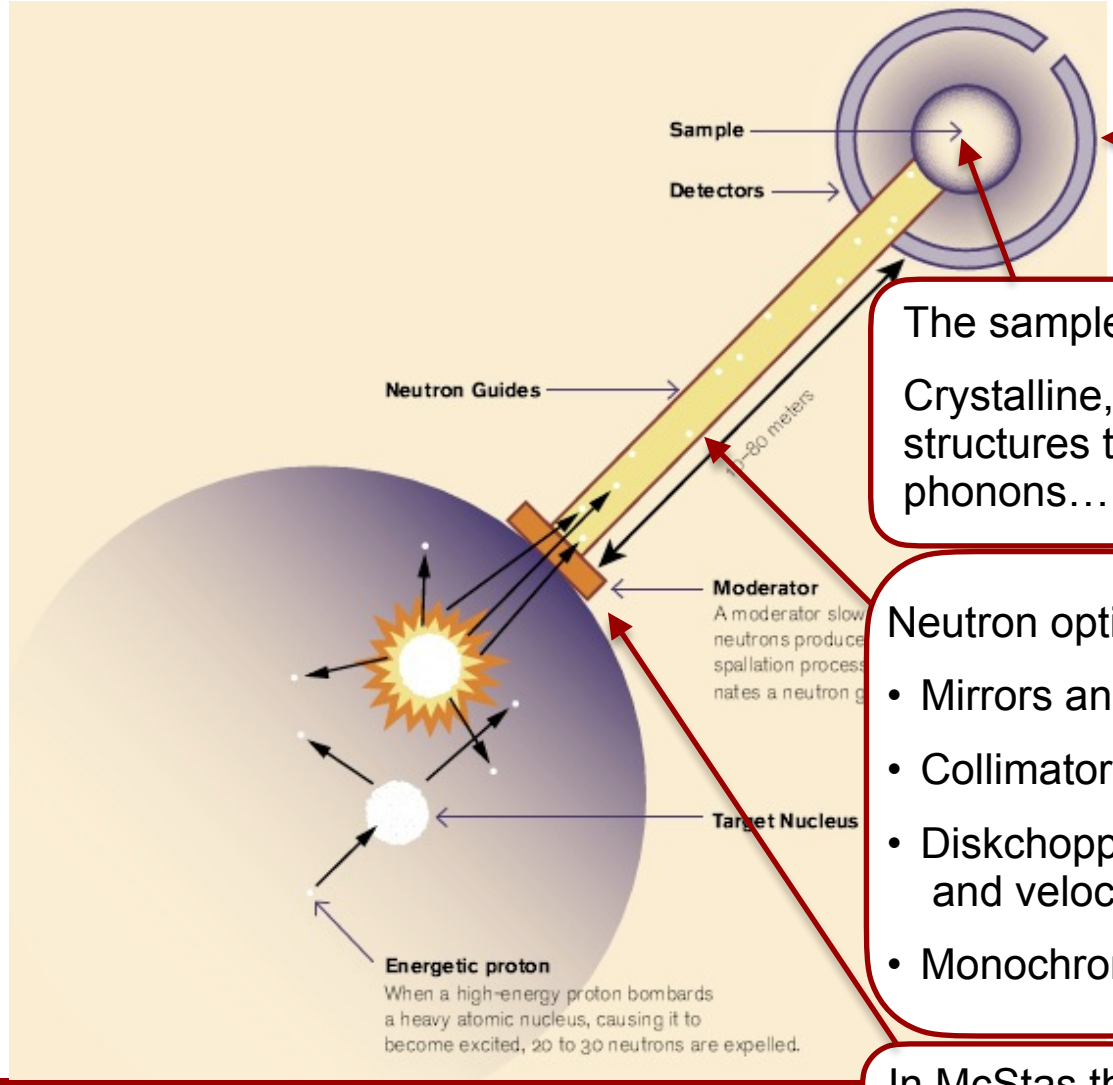
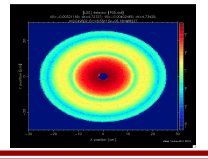
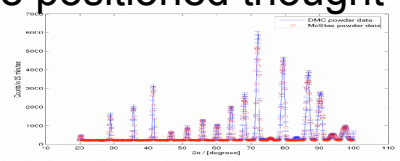


Detectors are “monitors” in McStas. Mostly they act as “perfect probes” and can be positioned thought your instrument gathering 1D/2D/ event lists…





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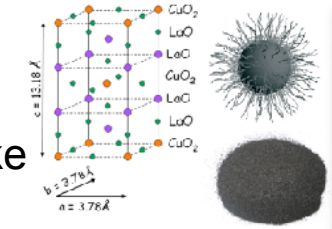

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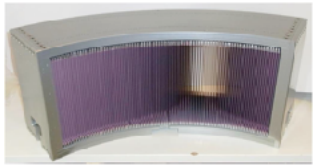
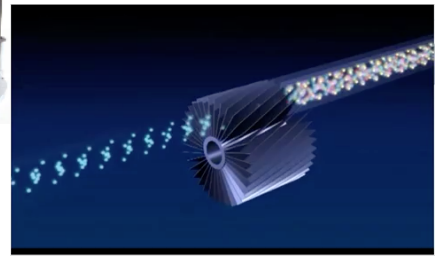
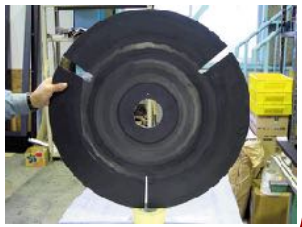






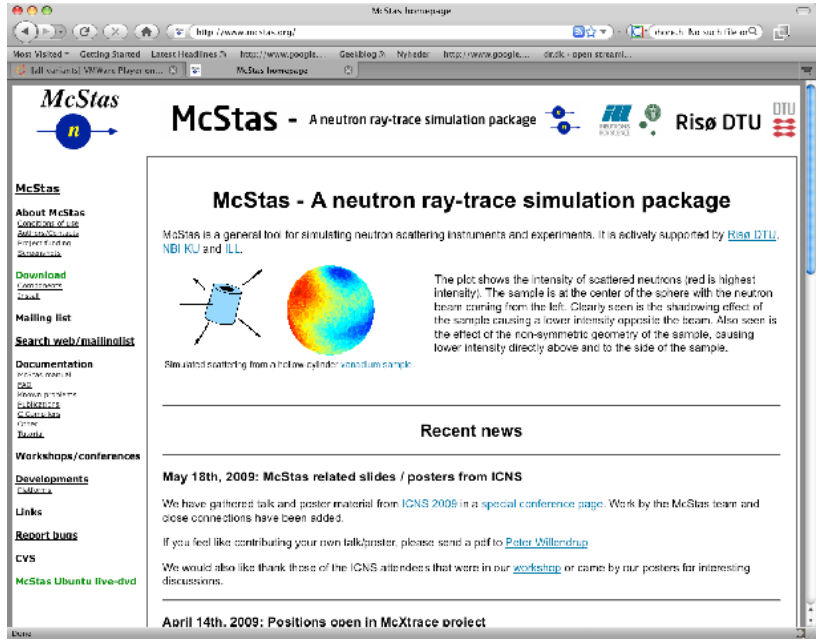
In McStas the moderator is the “source”

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 ~2-3 people full time plus students and user-contributions



Project website at

http://www.mcstas.org

mcstas-users@mcstas.org mailinglist

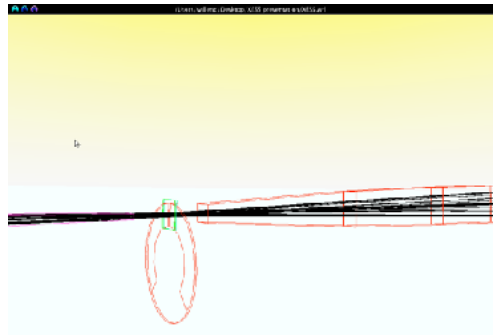
McStas Introduction

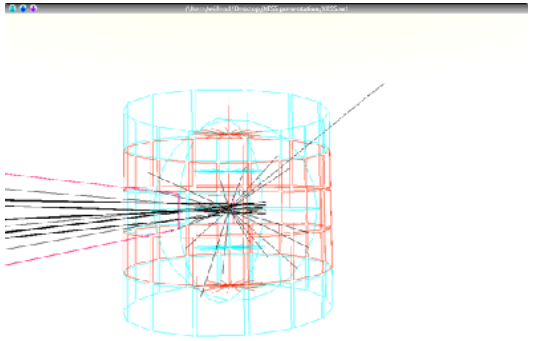
- Synergy, knowledge transfer, shared infrastructure

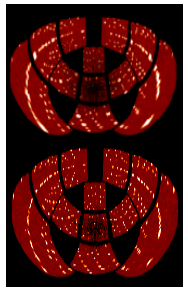
What is McStas used for?

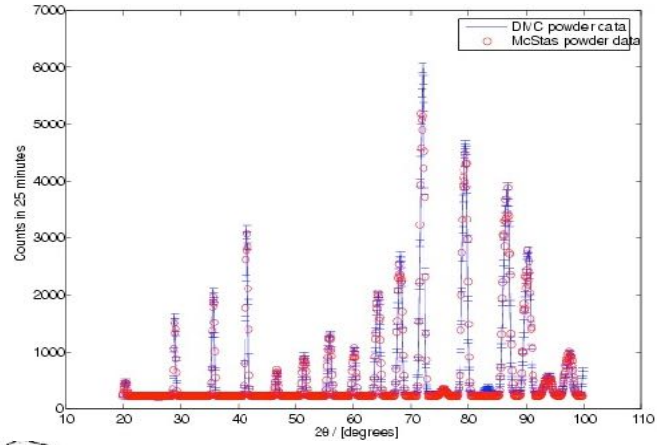
- Instrumentation
- Planning
- Construction
- Virtual experiments
- Data analysis
- Teaching

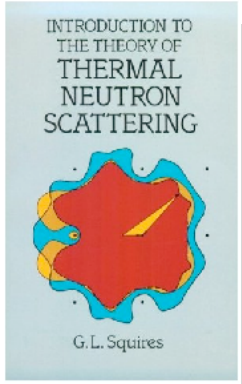
(KU, DTU)

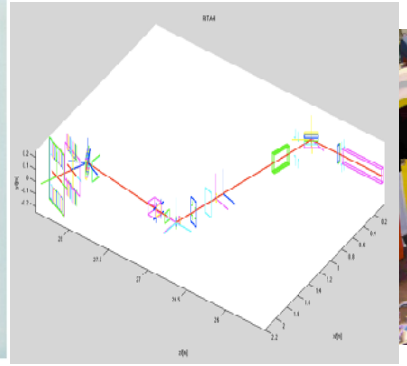


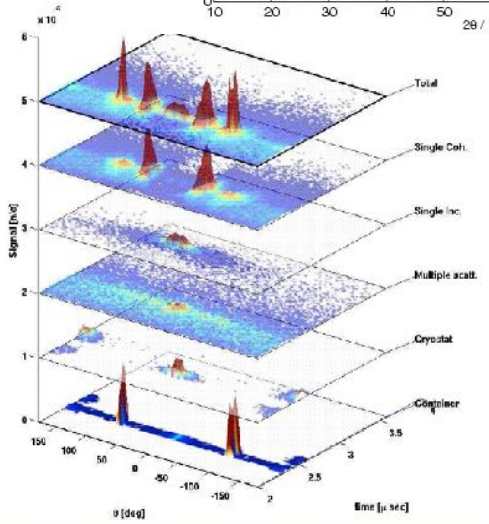












Reliability - cross comparisons

- 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

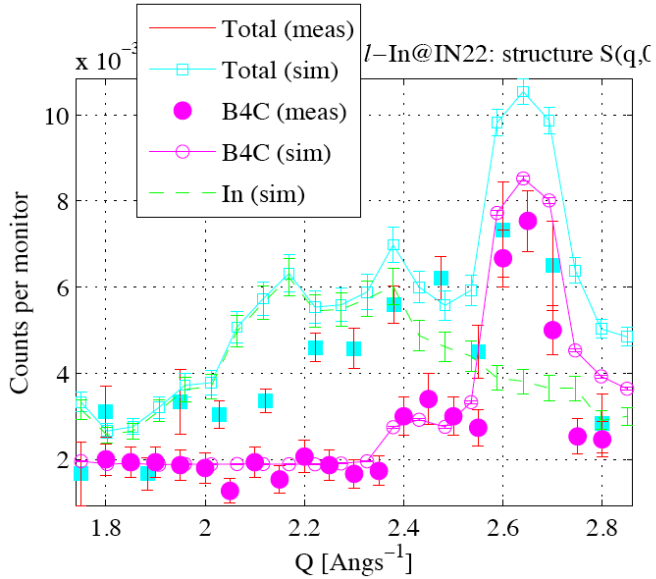
Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment
Volume 1063, June 2024, 169291

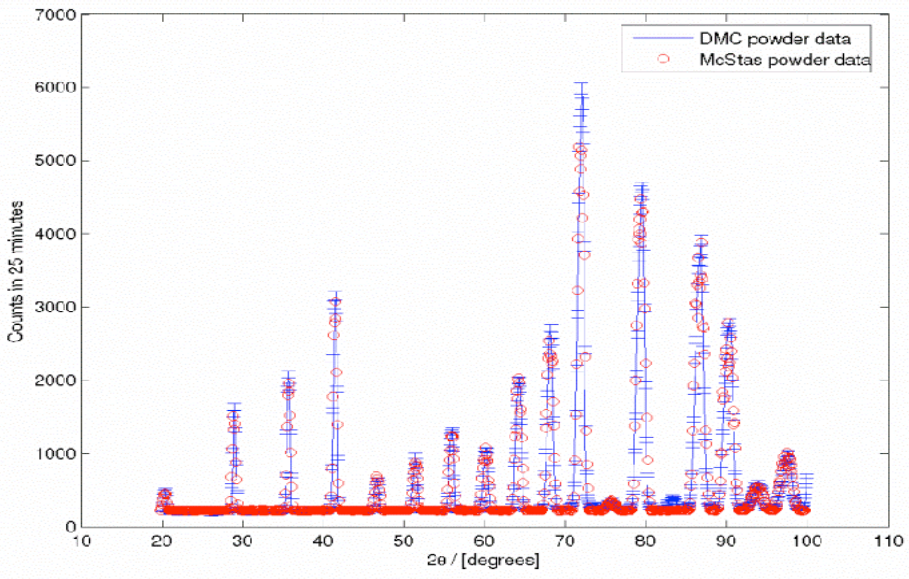
Full Length Article

Verification of the McStas code using two double axis neutron diffractometers

D. Potashnikov [a], A. Pesach [a], O. Rivin [a], O. Ozeri [b], Z. Yungrais [c], M. Bertelsen [d], E.N. Caspi [a]

https://doi.org/10.1016/j.nima.2024.169291





E. Farhi, P. Willendrup, from IN22 benchmark exp.

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

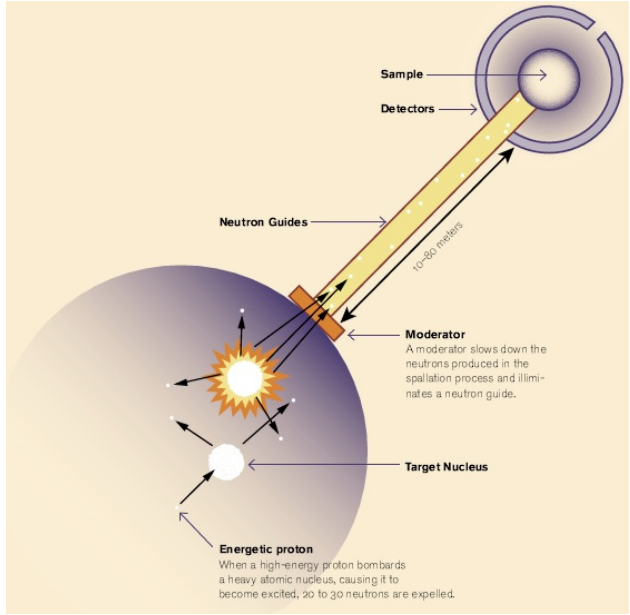
McStas overview

- Portable code (Unix/Linux/Mac/Windoze)
- Ran on everything from iPhone to 1000+ node cluster!

CPU's

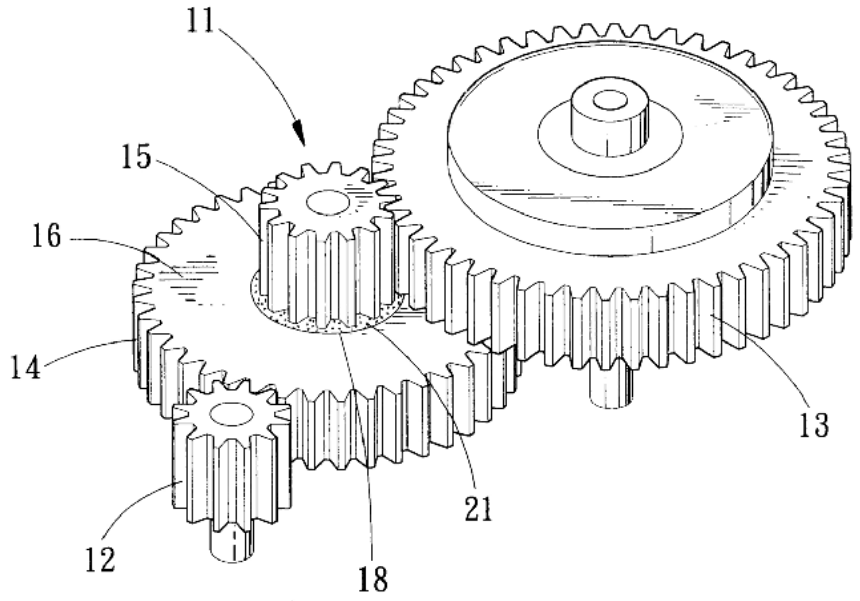
+ NVIDIA GPU's

- '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
  - ...

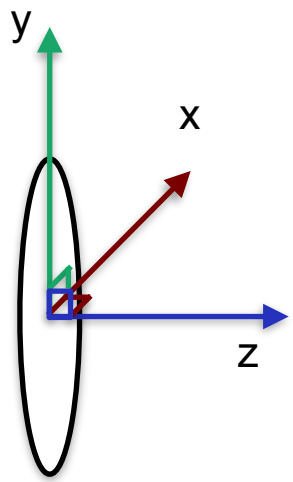


Implementation

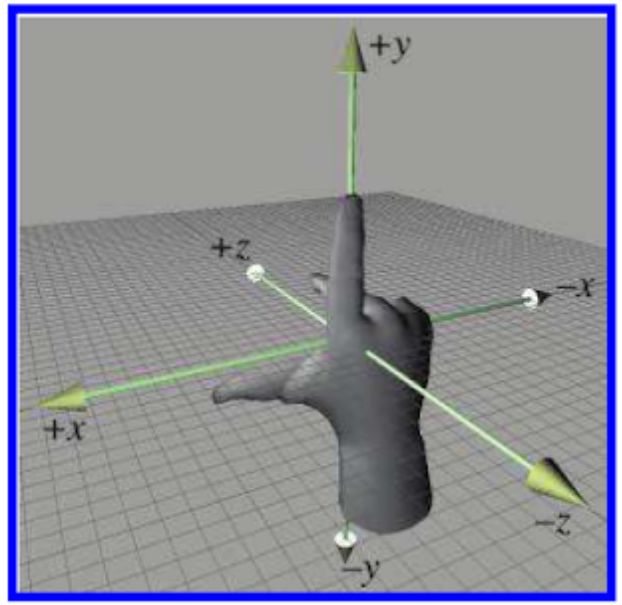
- Three levels of source code:
  - Instrument file (All users)
  - Component files (Some users)
  - ANSI c code (no users)

Placing components - source

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



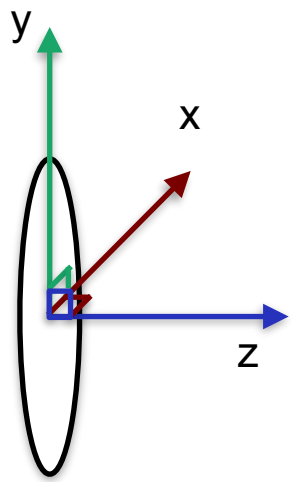
- z is along neutron beam direction
- y is vertical
- x at an angle of 90° wrt. z,y



Right-handed coordinate system

Placing components - source

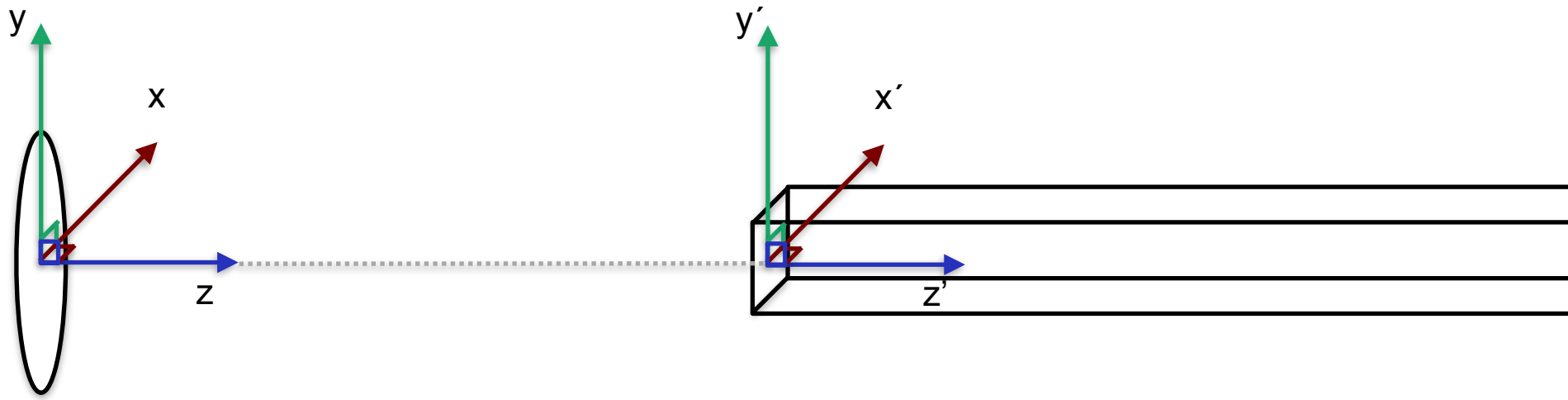
- Often the source coordinate system coincides with the “lab” coordinate system, denoted ABSOLUTE in McStas language, i.e.



- 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**

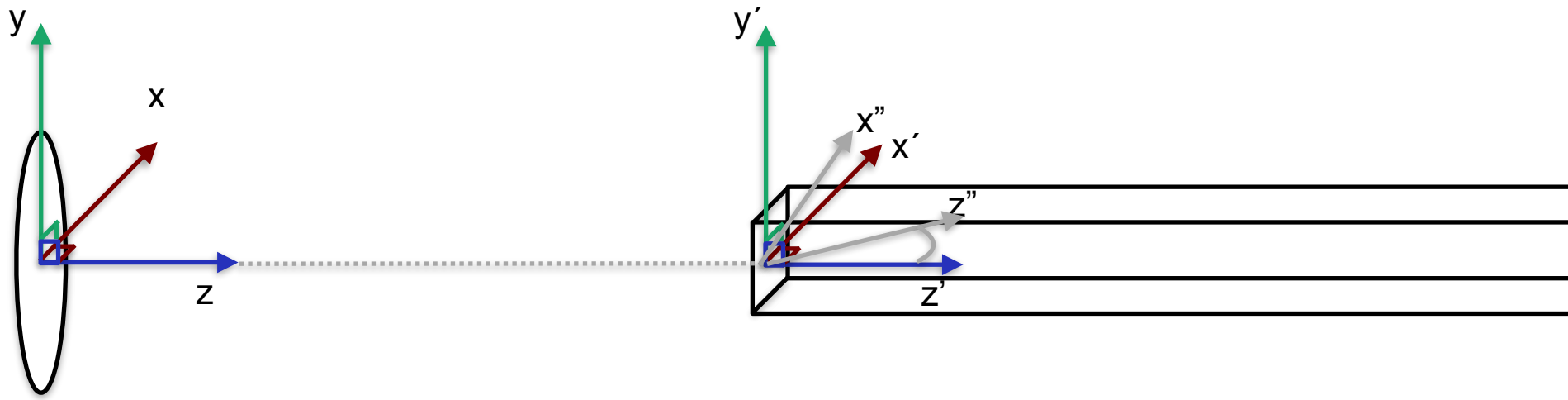


COMPONENT Source = Source_simple(…)
AT (0,0,0) ABSOLUTE

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**

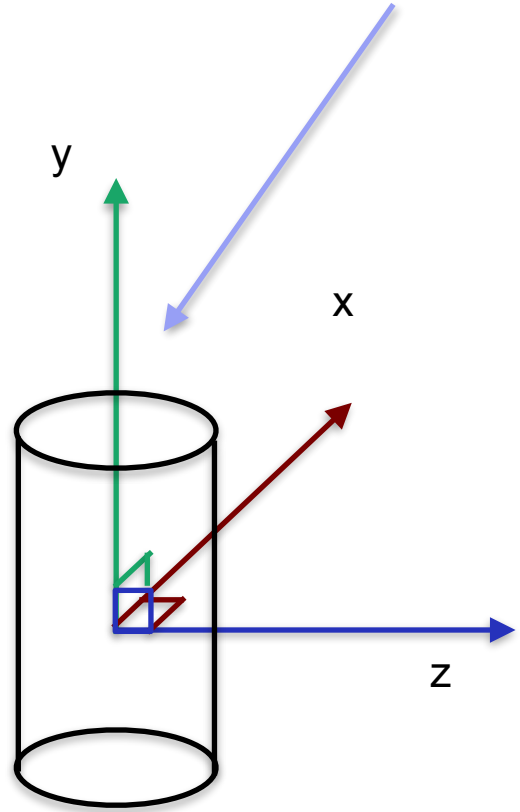


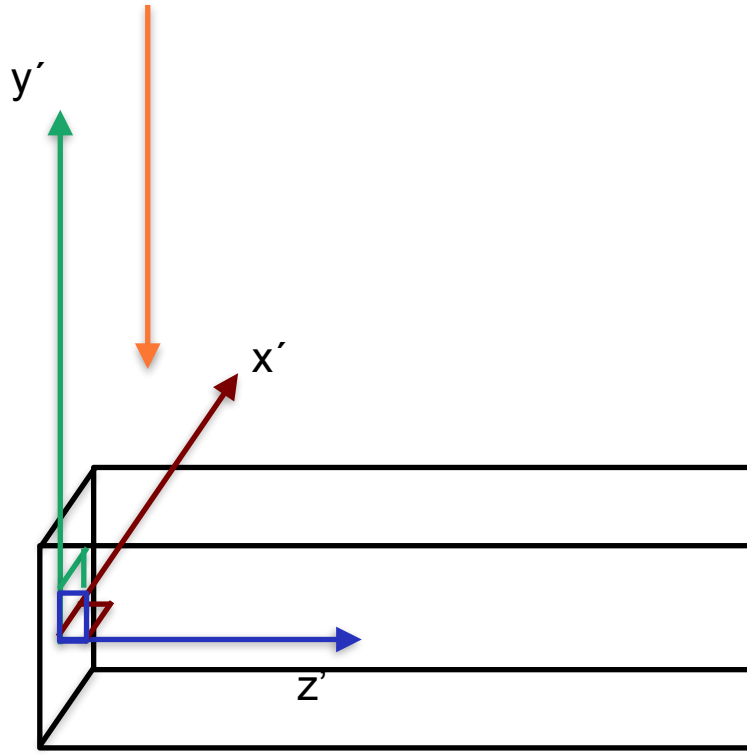
COMPONENT Source = Source_simple(…)
AT (0,0,0) ABSOLUTE

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.)

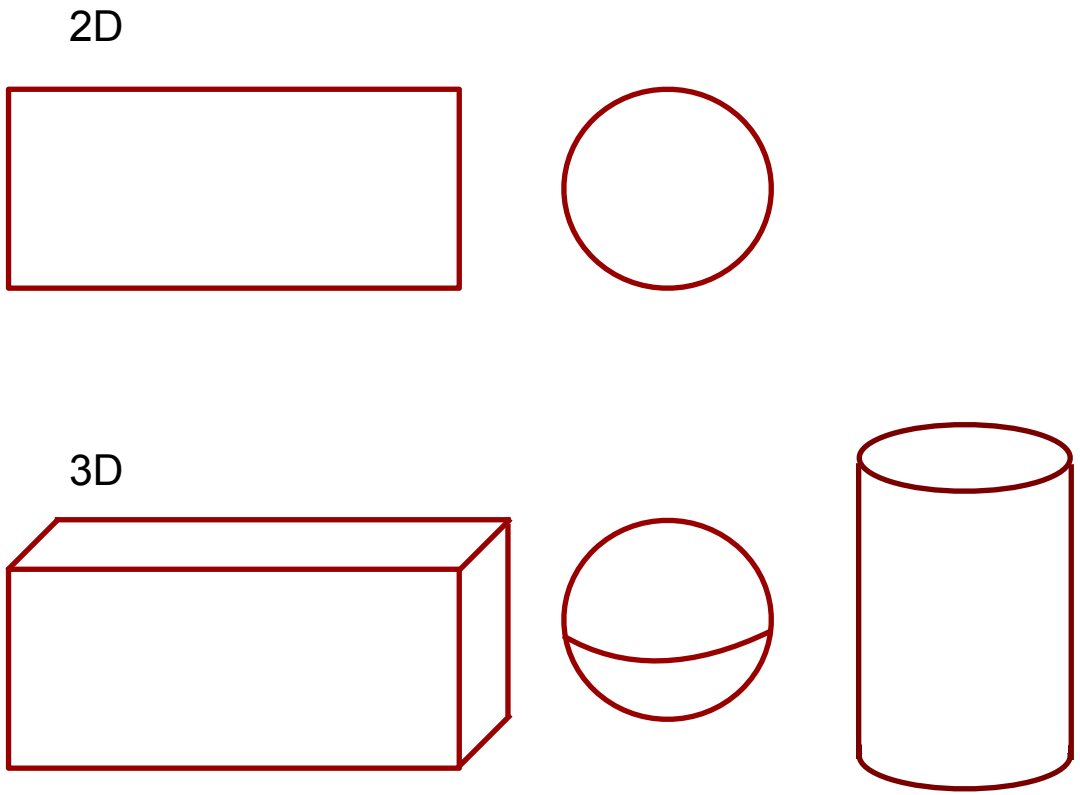
Components often have their origin at the centre of mass, i.e. for samples … but not for neutron guides

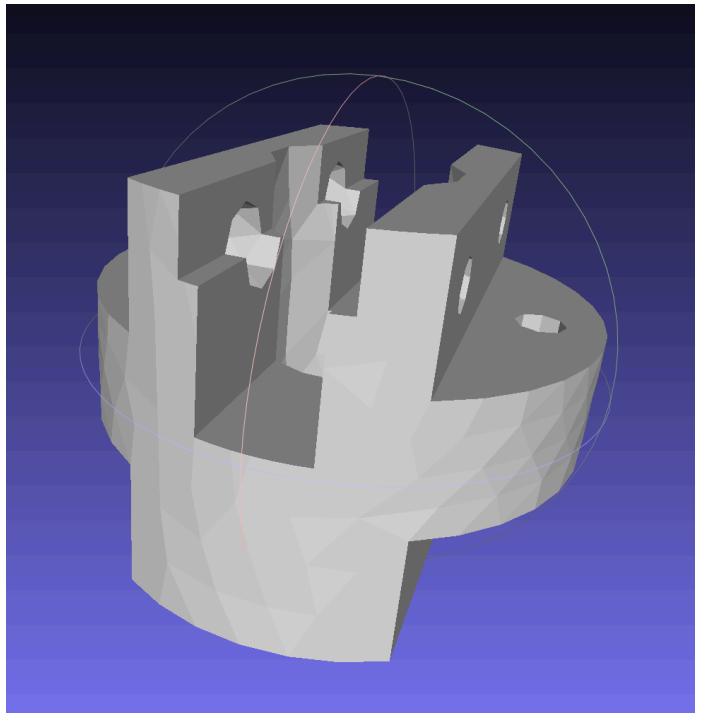




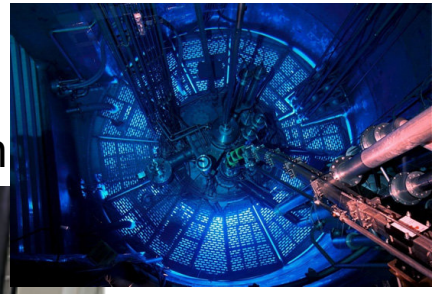
Generally speaking, the component author can choose
the meaningful coordinate system for the given problem!
- The McStas system takes care of the transformation between them….

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

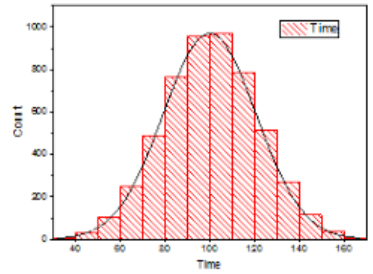




Component classes



- 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

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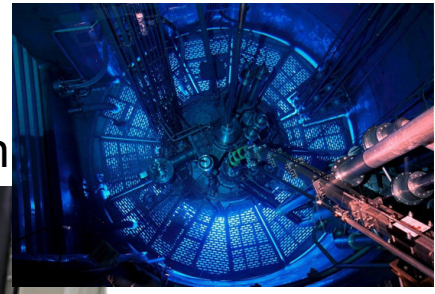
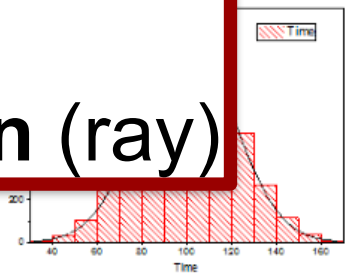


Common to all components:

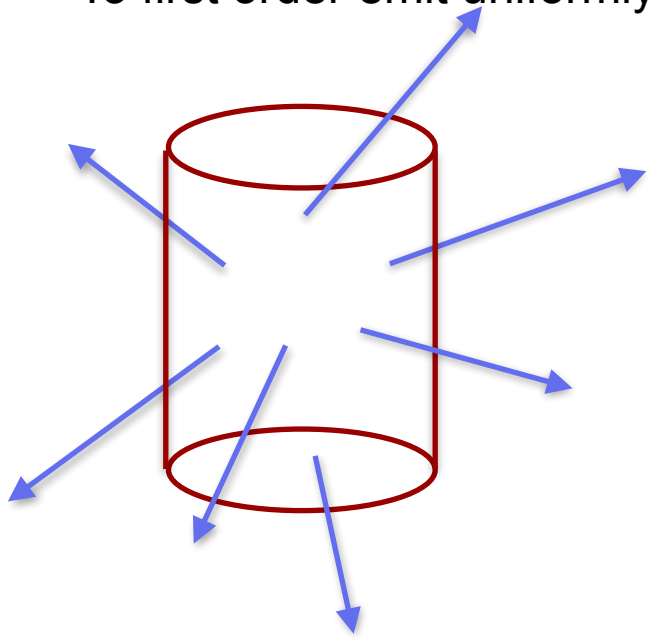
They set, manipulate/interact with

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

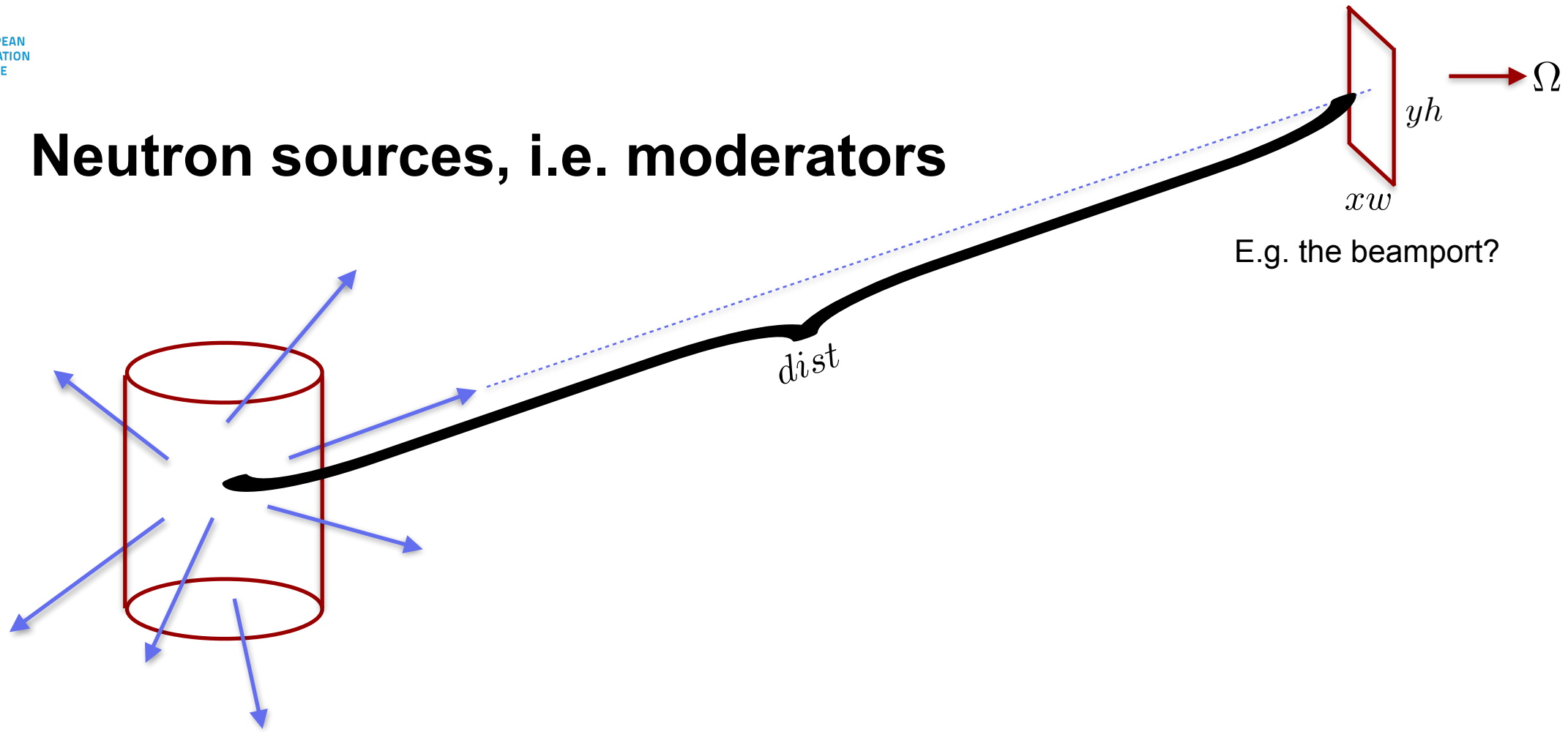


Neutron sources, i.e. moderators

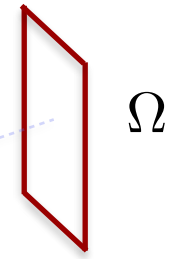
- To first order emit uniformly into 4π steradian



Neutron sources, i.e. moderators

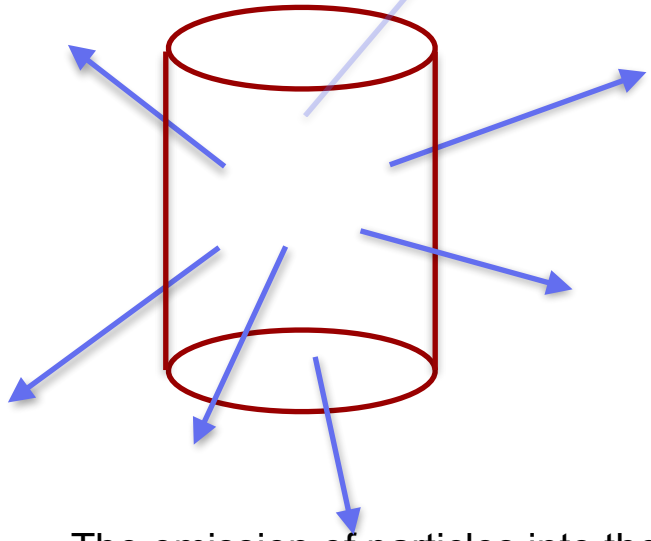


- Generally we are intersted in the input to a single instrument, characterised by a certain solid angle Ω, often corresponding to a rectangle xwx yh at a distance $dist$ from the source



Neutron sources, i.e. moderators

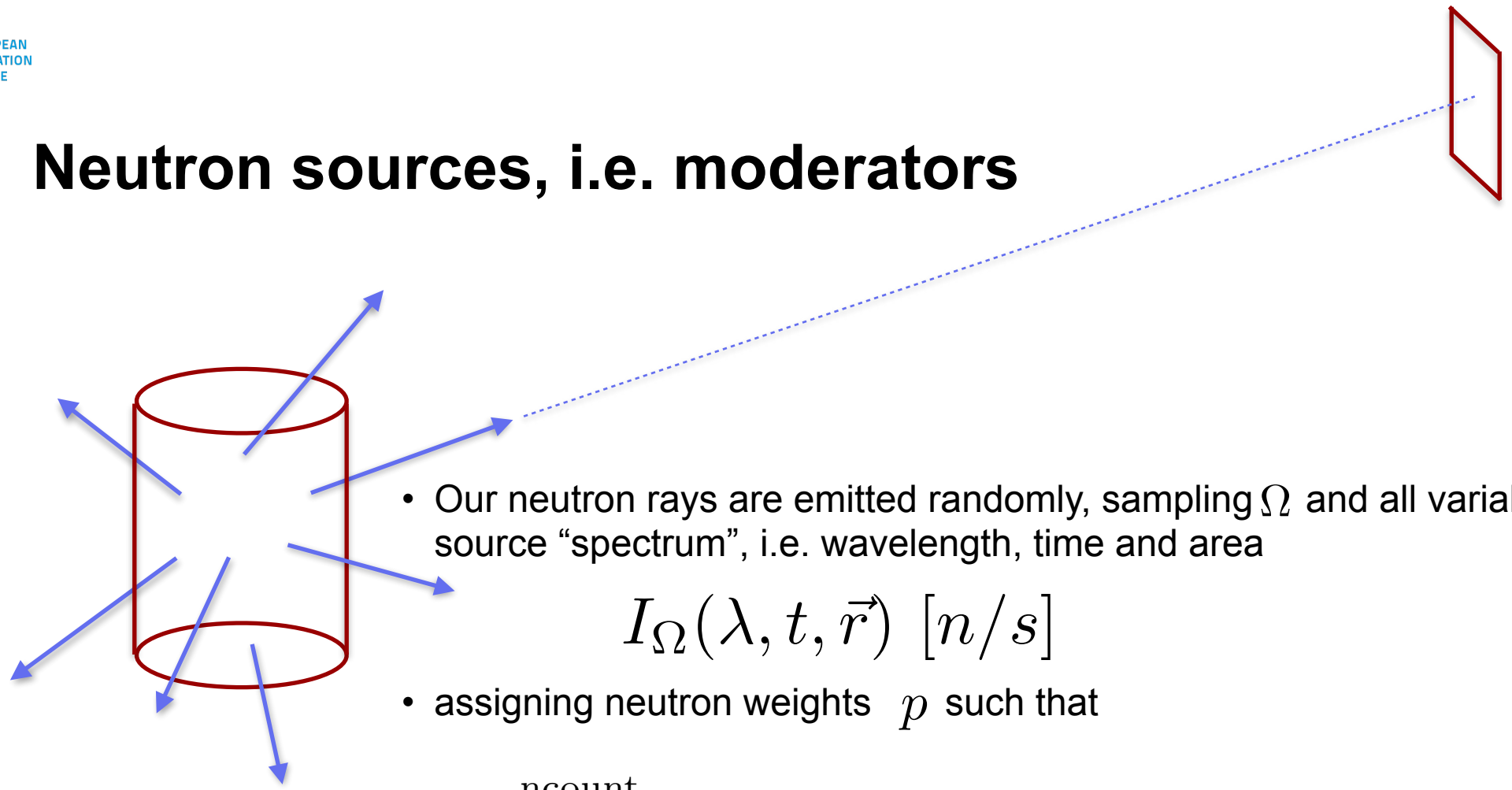
- The emmission intensity into our chosen solid angle Ω can be a function of wavelength, time (pulsed sources) and possibly point of origin on the source surface



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

- 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

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

Neutron rays in McStas - what are they?

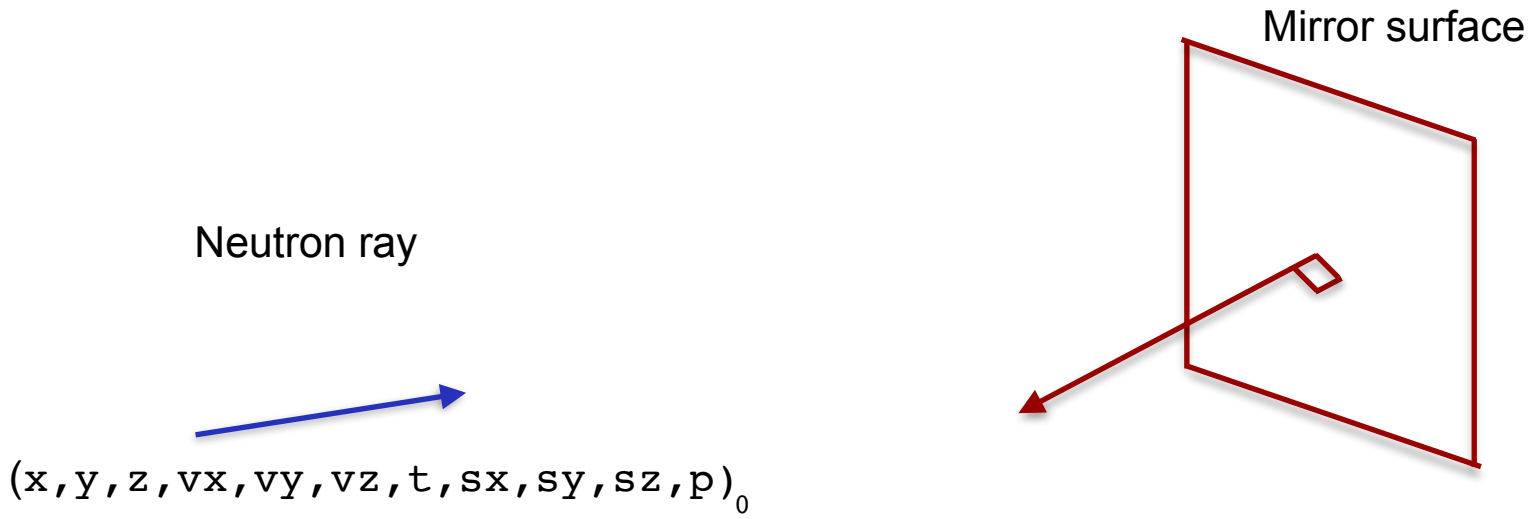
Neutron **ray** in McStas:	
Location	`x,y,z`
Velocity	`vx,vy,vz`
Time	`t`
Polarisation.	`sx,sy,sz`
Intensity	`p`

- 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`)

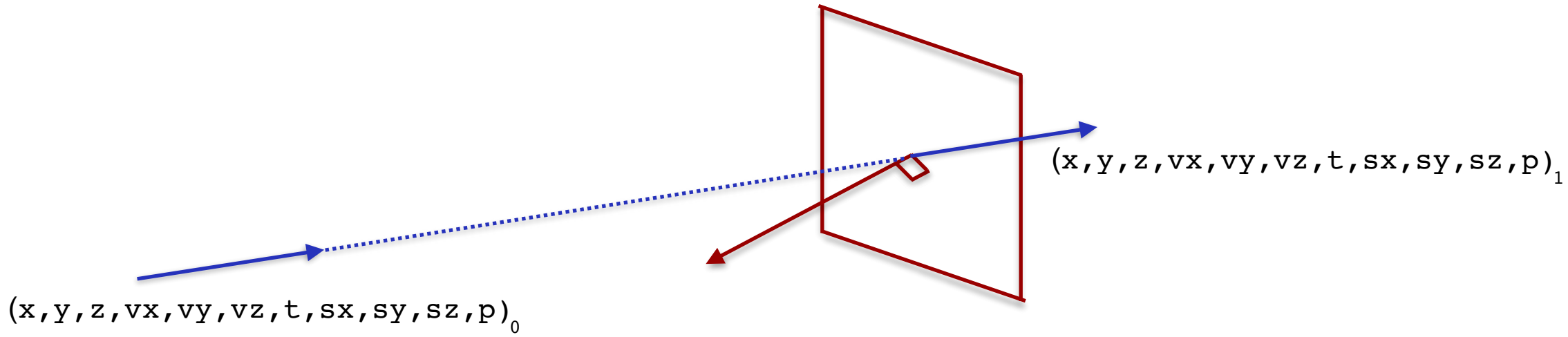
Neutron (ray)-matter interaction 1: reflecting surface

- 1 starting situation



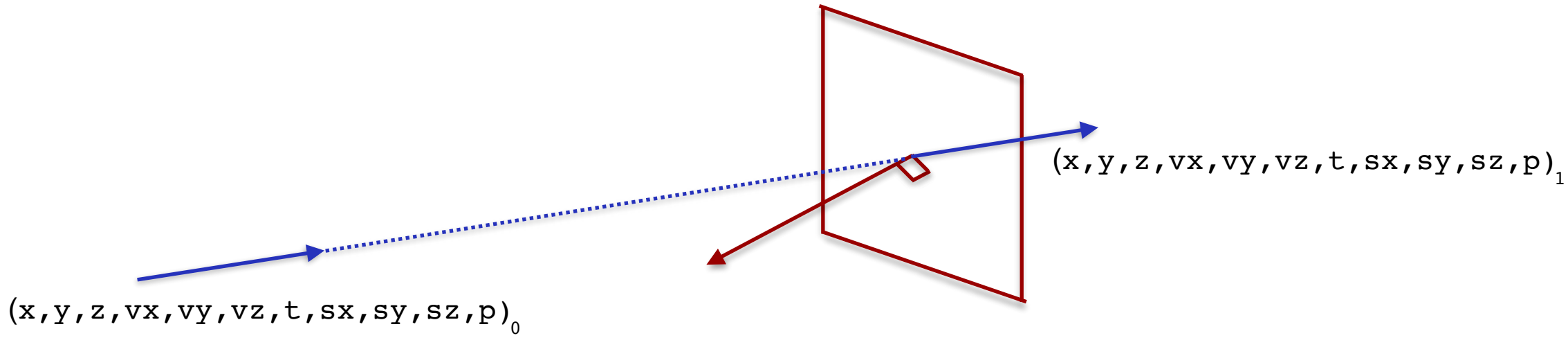
Neutron (ray)-matter interaction 1: reflecting surface

- 2. Propagate to the mirror surface



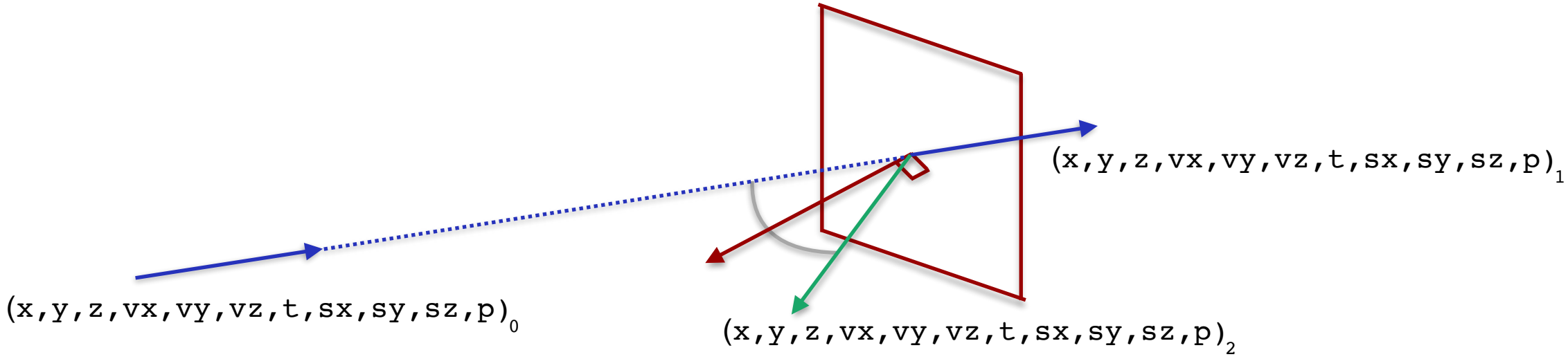
Neutron (ray)-matter interaction 1: reflecting surface

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



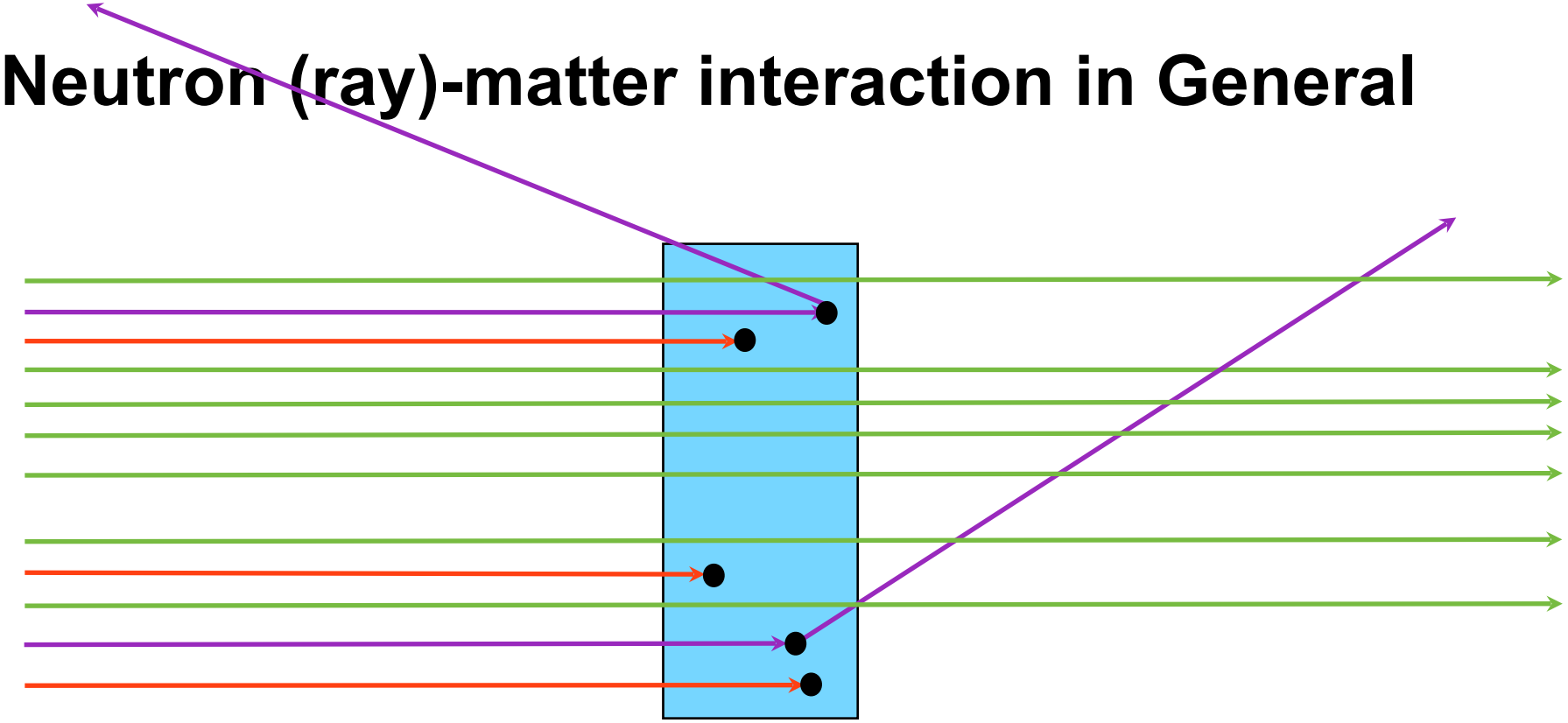
Neutron (ray)-matter interaction 1: reflecting surface

- 4. Reflect



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

Neutron (ray)-matter interaction in General



A neutron hitting a sample can be:
absorbed, transmitted, or scattered

Samples

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

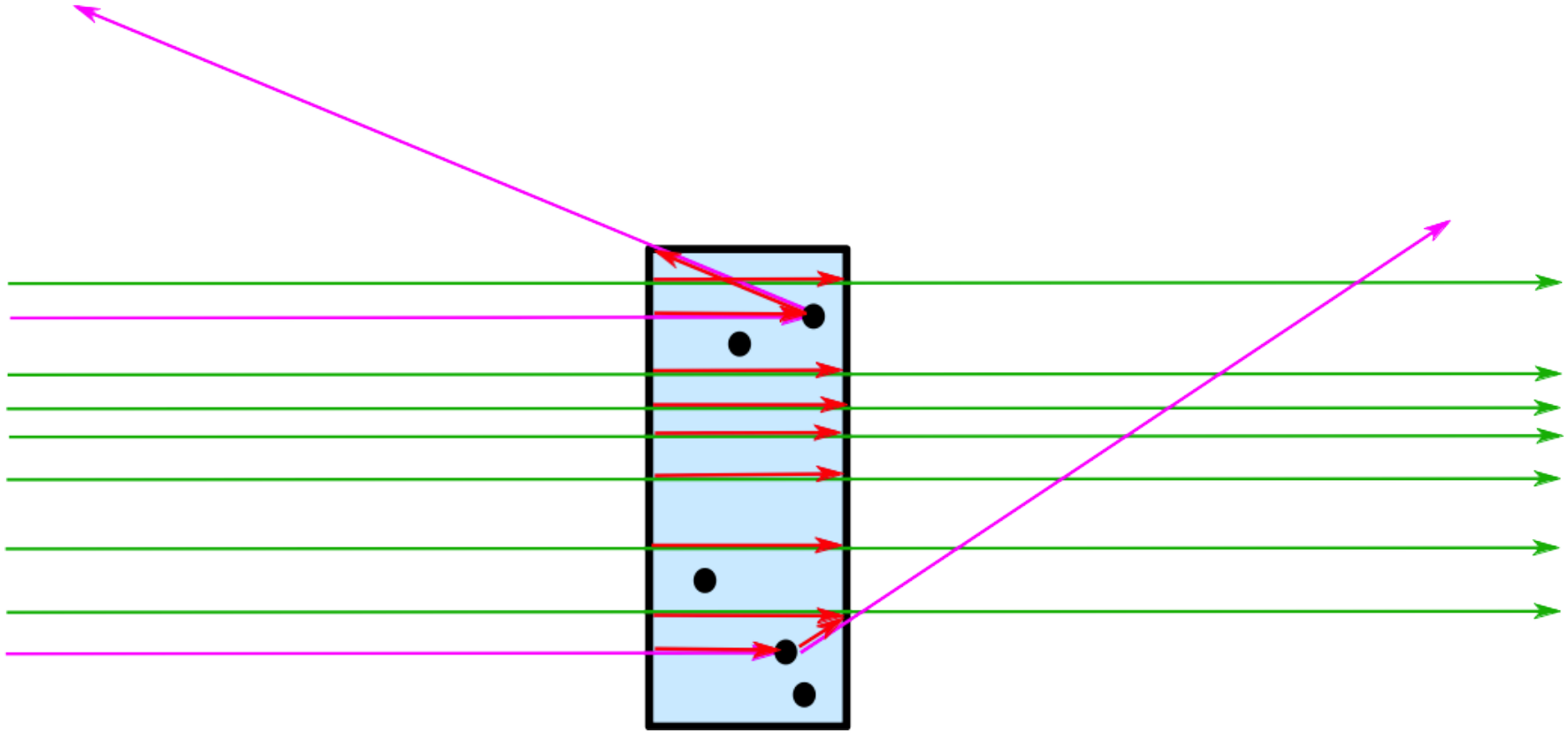
$$\Sigma_* = \rho \sigma_*$$

macroscopic cross section [cm^{-1}]

number density [$atoms/cm^3$]

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

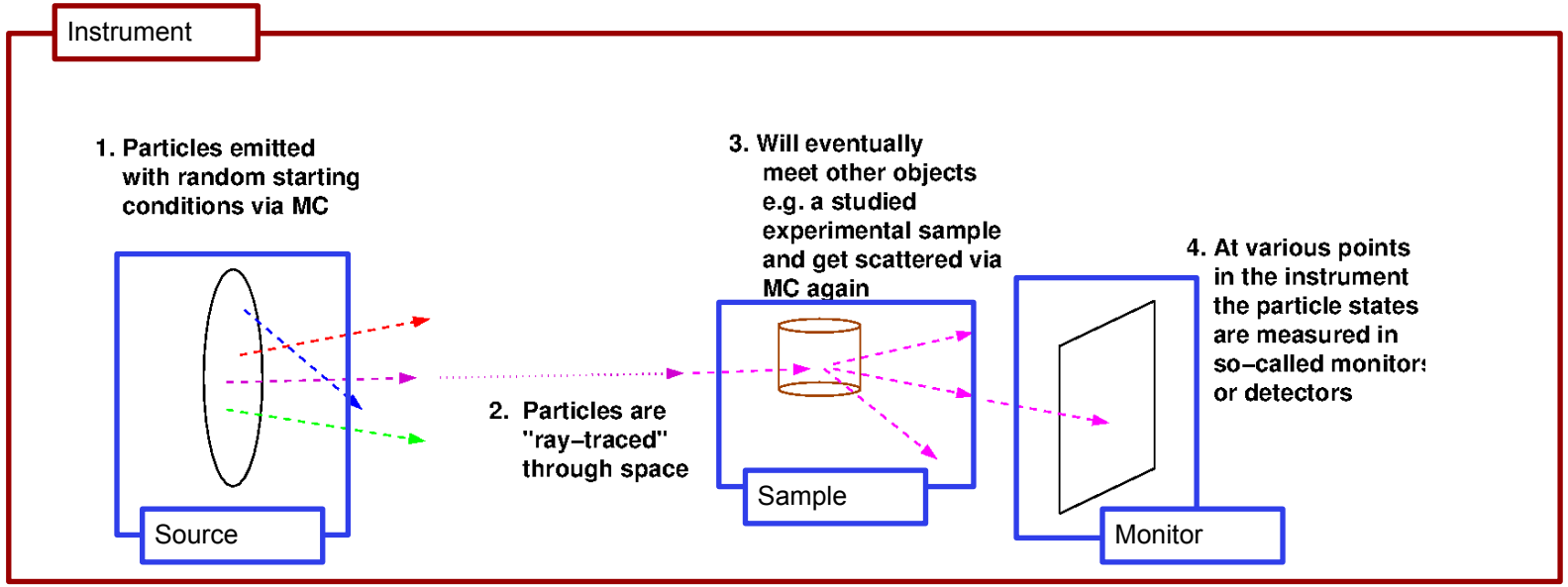
Samples/Matter interaction in General in McStas



A neutron ray hitting a sample can be:
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

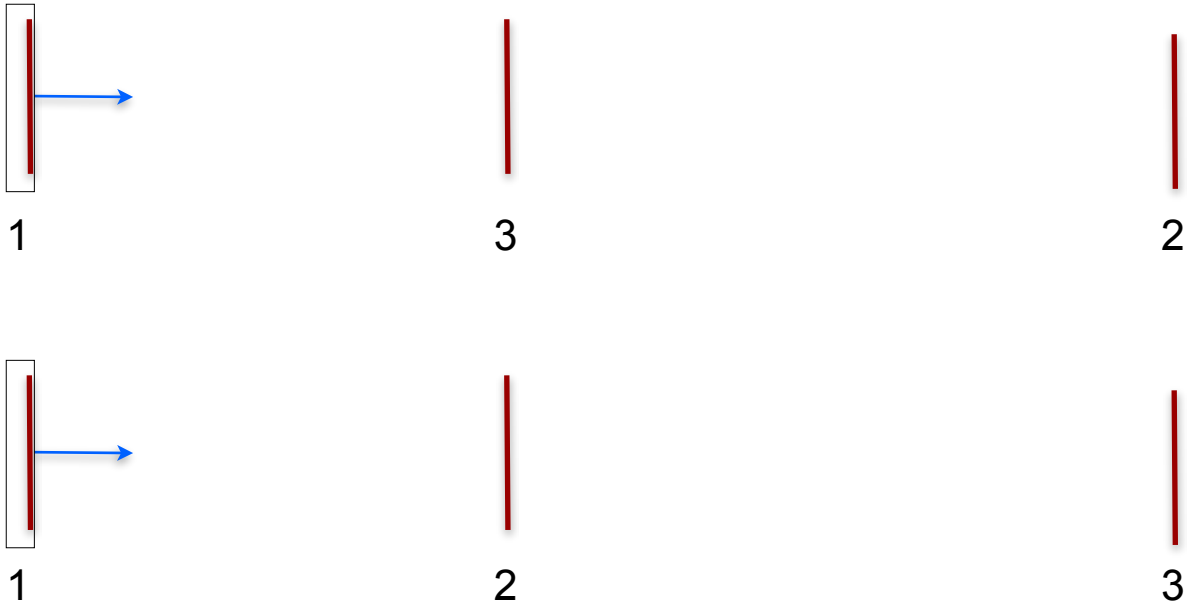
$$p_j = w_j p_{j-1}$$

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

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.

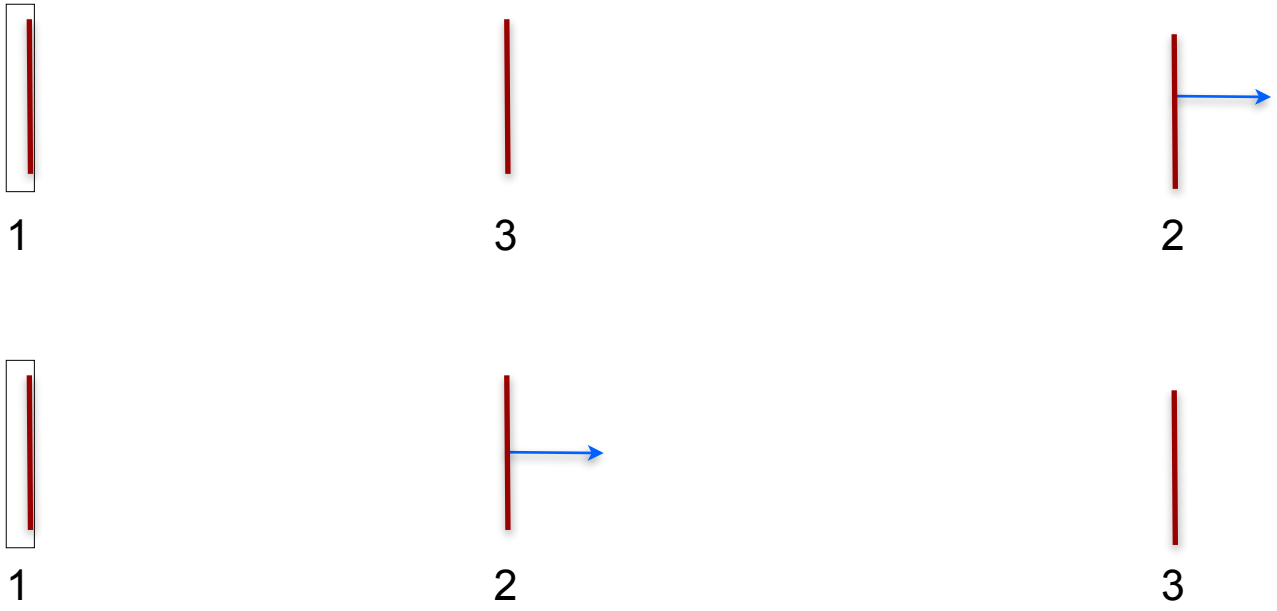
In case of "branching", i.e. multiple outcomes, it is clear that $\sum_b f_{\mathrm{MC,b}} = 1$

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



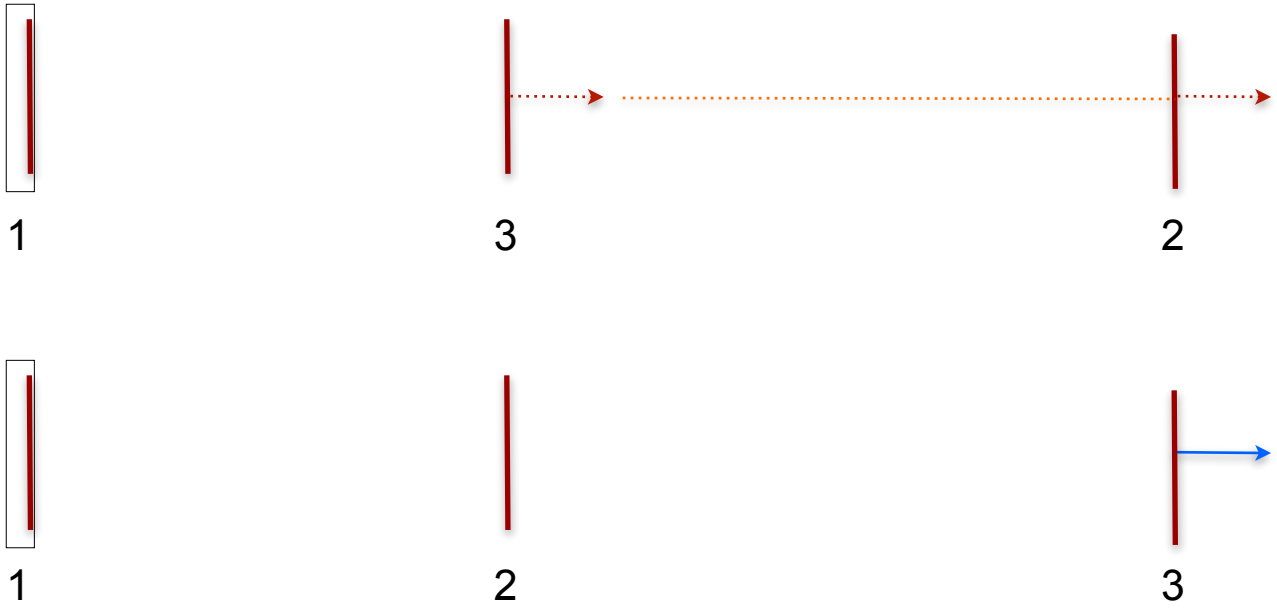
Starting at the source

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



Moving to first comp in the list

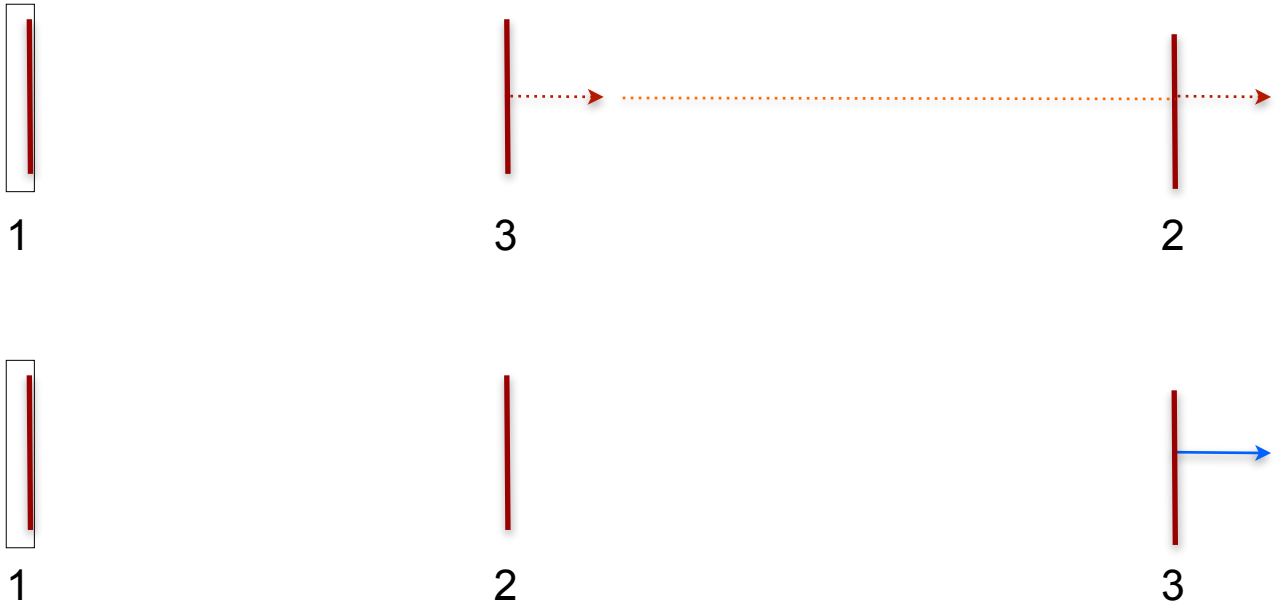
To first order, McStas is linear and follows sequence of components in your file…



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

Default behavior is to ABSORB this type of neutron.

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



The order of components is important,

and in general overlaps should be avoided!

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

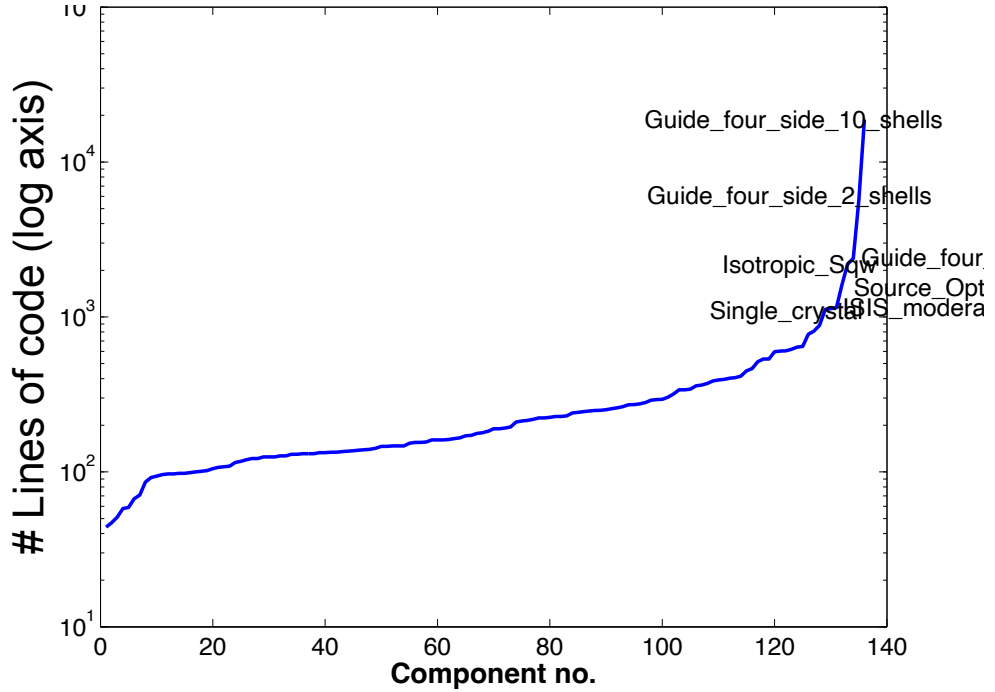
Default behavior is to ABSORB this type of neutron.

(Special case: To avoid that ABSORB let monitors use restore_neutron=1)

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 - 240 comps in total



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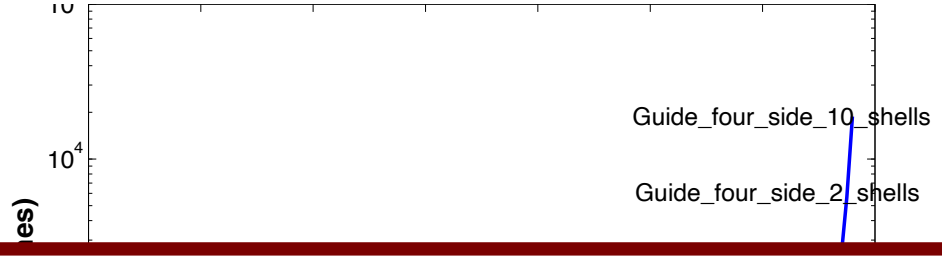
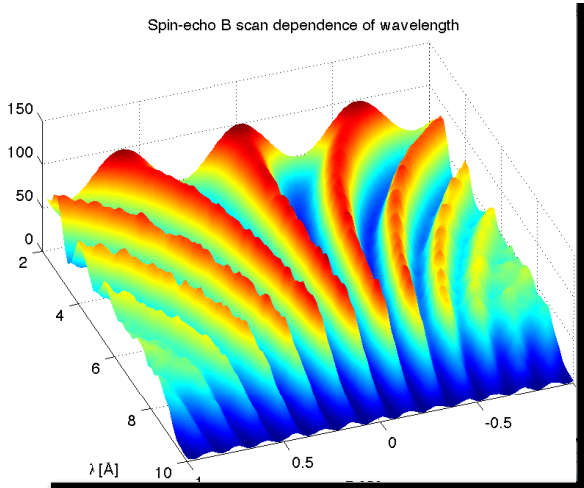
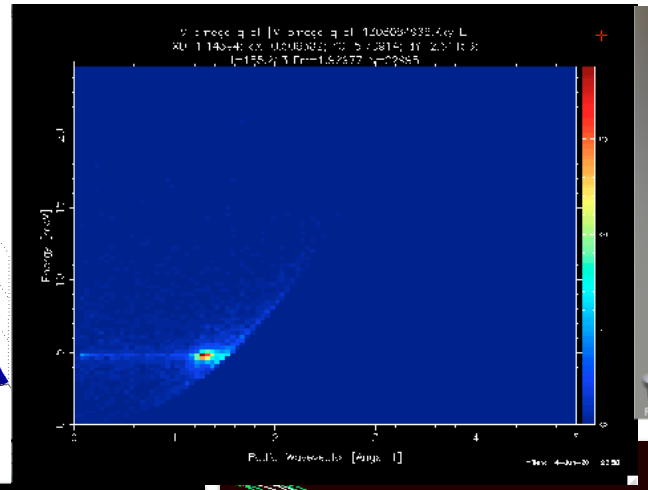
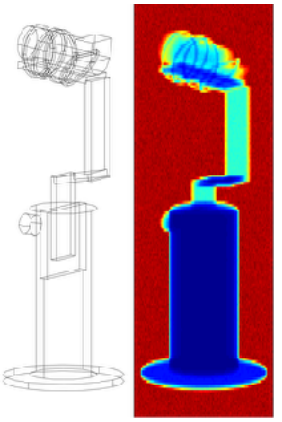


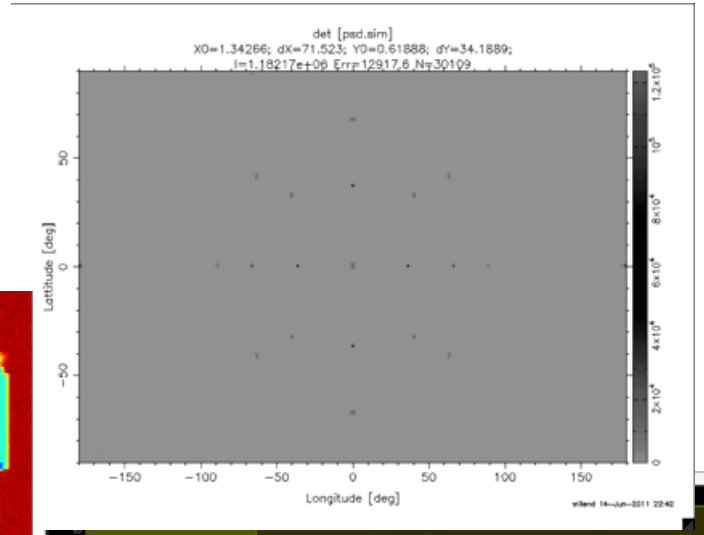
- Well-developed community support
  - –30-40% of existing and new additions are from users
  - –No direct refereeing of the code, but these requirements:
    - –At least one test-instrument
    - –Meaningful documentation headers (in-code docs)
  - –Contributions go in dedicated contrib/ section of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

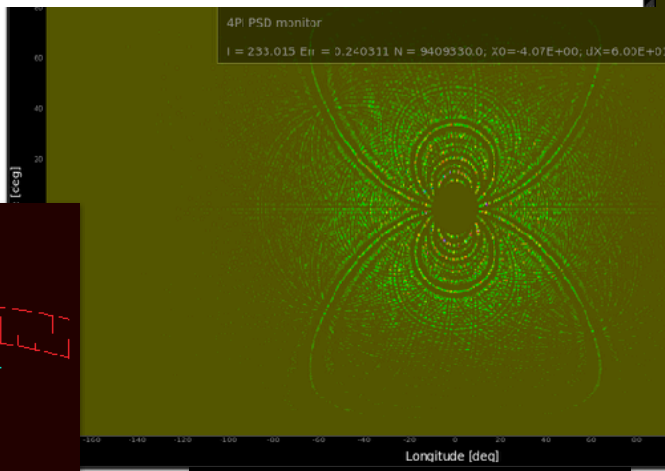
Example suite: ~252 instruments

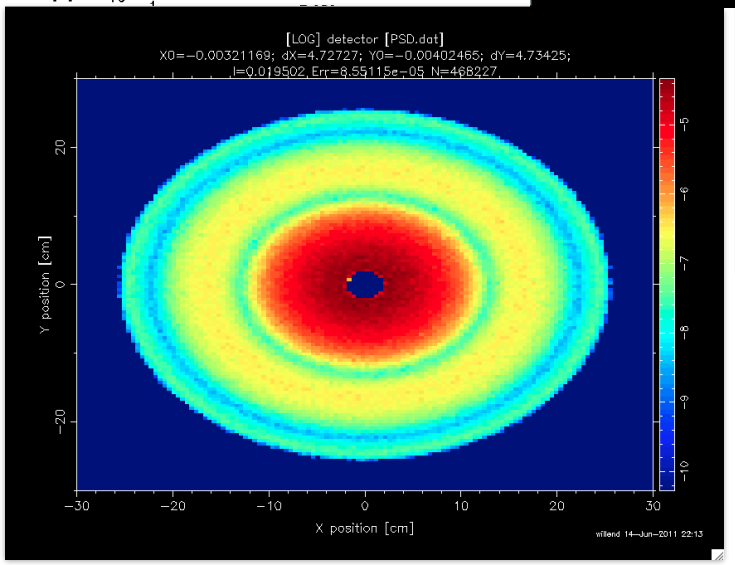


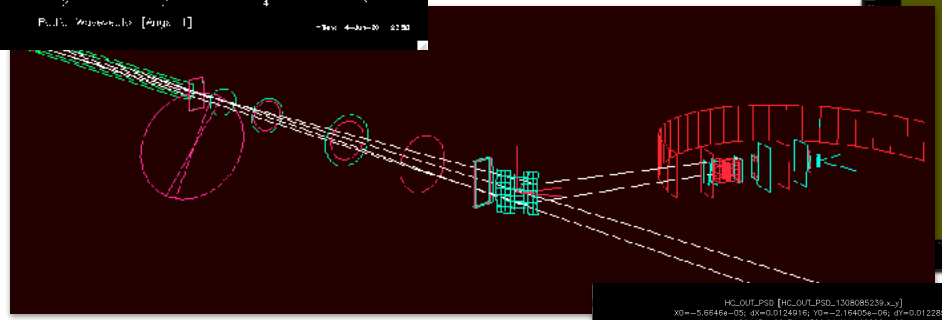


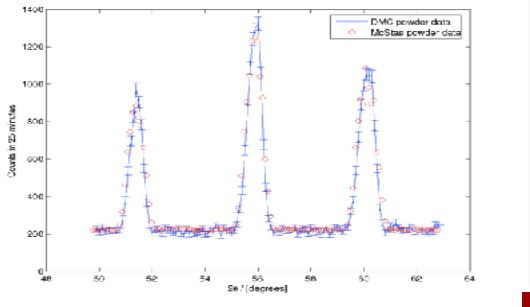


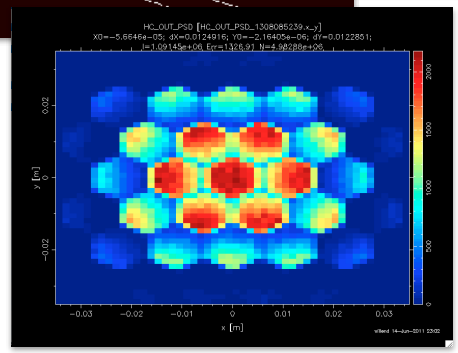


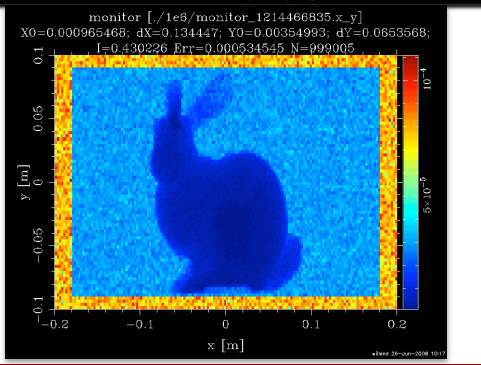






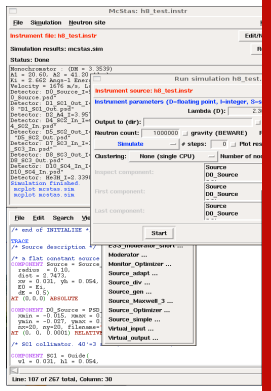


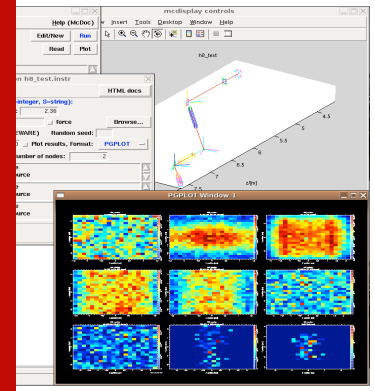




DTU

EUROPEAN SPALLATION SOURCE





THIS IS NOT THE END

IT'S JUST THE BEGINNING