CSNS McStas training
March 25th-29th 2019

2019 CSNS McStas School

McStas

Agenda

- A (very) brief introduction to neutrons, Monte Carlo & raytracing
- Components of neutron instruments
- How McStas works under the hood
- Components and instruments
- A demo

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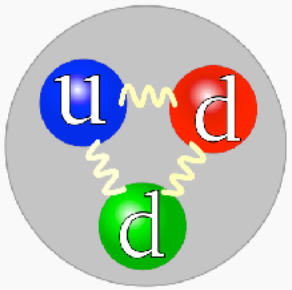
McStas: Neutrons, Monte Carlo & ray-tracing

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) ×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 ×10^{-26} e·cm
Electric polarizability	1.16(15) ×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

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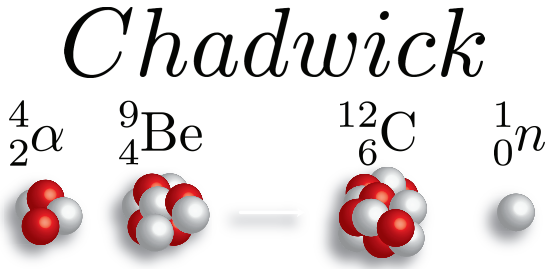
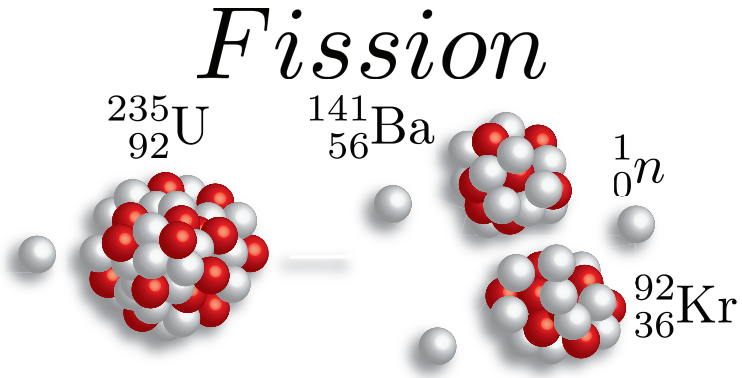
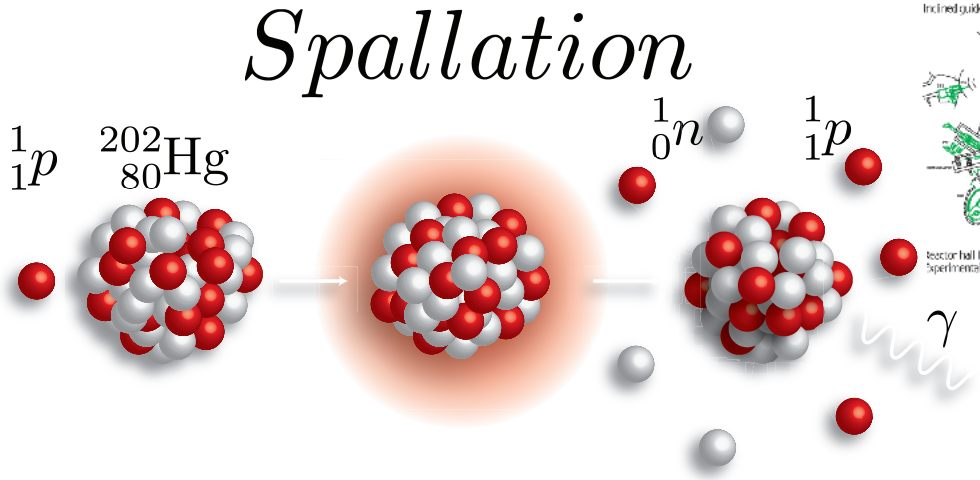
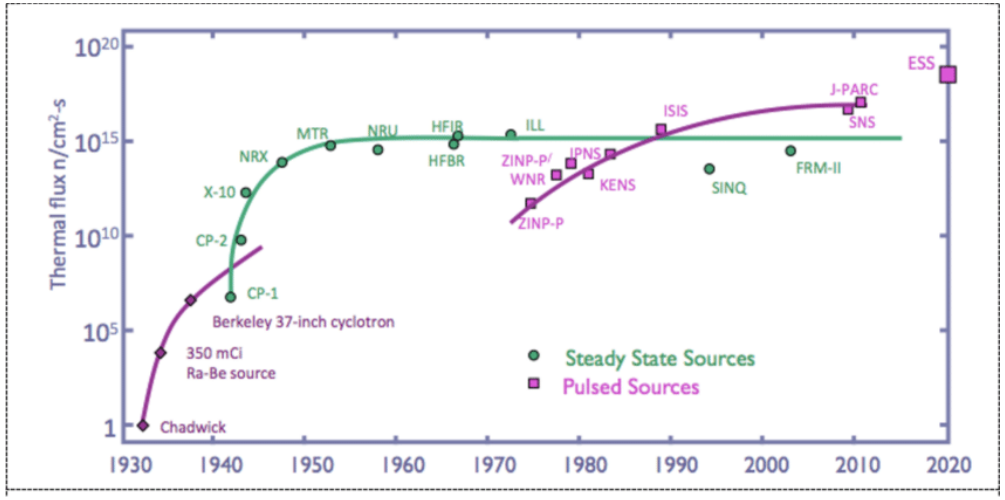
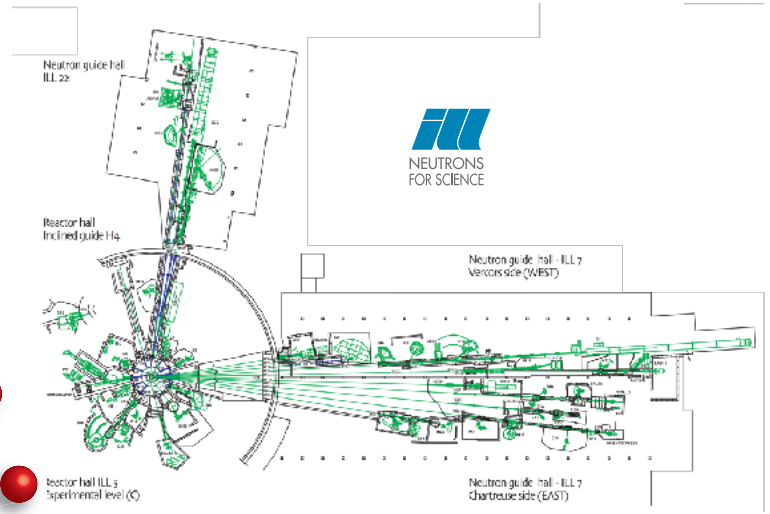
Neutron facilities

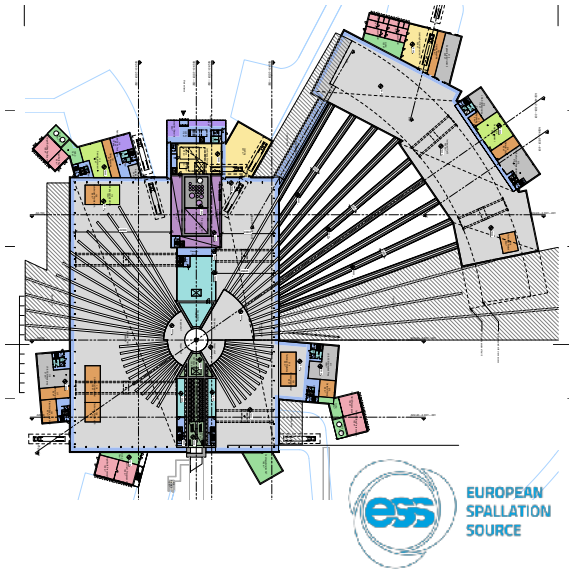












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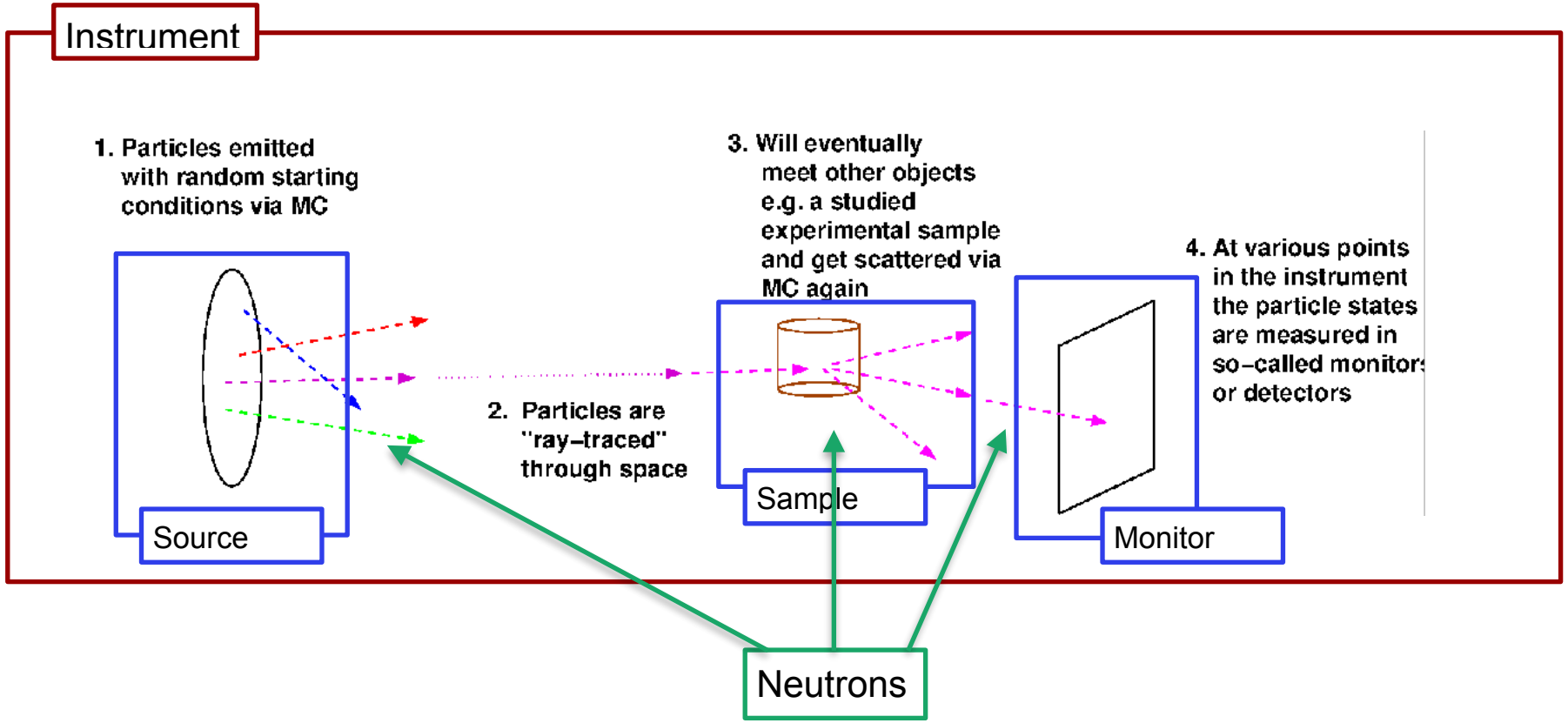
McStas

McStas is a Monte Carlo ray-tracer



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Origin of Monte Carlo methods

First application using computers:

Metropolis, Ulam and Von Neumann at Los Alamos, 1943

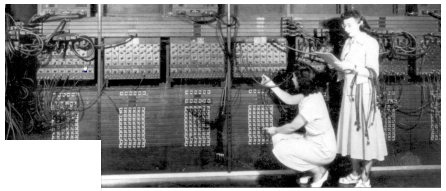
Neutron Scattering and Absorption in U and Pu, Origin of MCNP



Name:

Monte Carlo casino, a random generator (Ulam's father played poker)

Bradbury Science Museum, LANL



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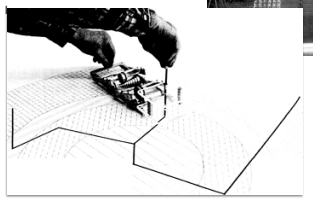

FERMIAC

US Army BRL → UPENN

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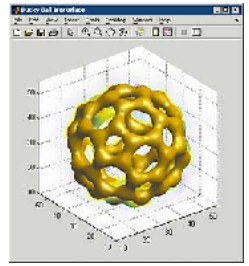
When to use Monte Carlo methods



Dimensionality of phase space must be large ($d > 5$)

Overall complexity is beyond reasonable analytical methods

Each event can be computed easily and independently MC is the '*lazy guy*' method – think microscopic

Examples:

Estimate π from a circle/square ("*Buffon needle*")

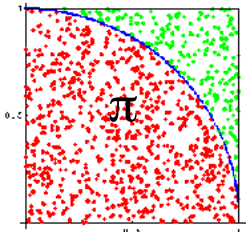
Area under/inside a curve/volume (integration)

Molecular Dynamics

spin-system phase transitions (*Ising* model)

nuclear reactions

ray-tracing (light, particles)



Number of points for which

$\{ x^2+y^2 \leq 1, (x,y) \in [0,1] \}$

Ratio circle/square → $\pi/4$

中国散裂中子源

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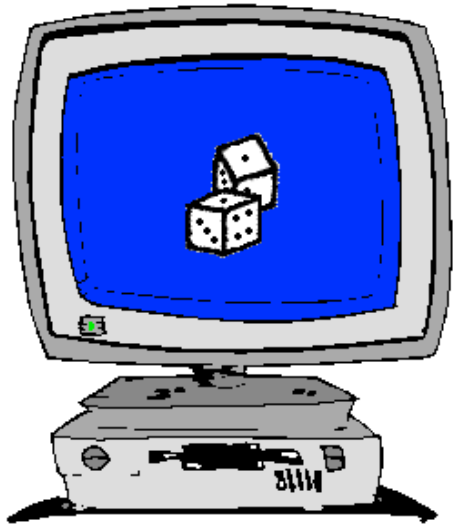
How to implement Monte Carlo methods ?

Good random generator:

from thermal electronic noise (hardware)

or quasi-random generators => *quasi*-Monte-Carlo

We encounter a probability $0 < p < 1$.



Crude Monte-Carlo (yes/no choice):

We shoot *n* events $\xi \in [0,1]$

We keep events that satisfy $\xi < p$

***np* events low statistics**

Importance sampling (fuzzy choice – event weighting):

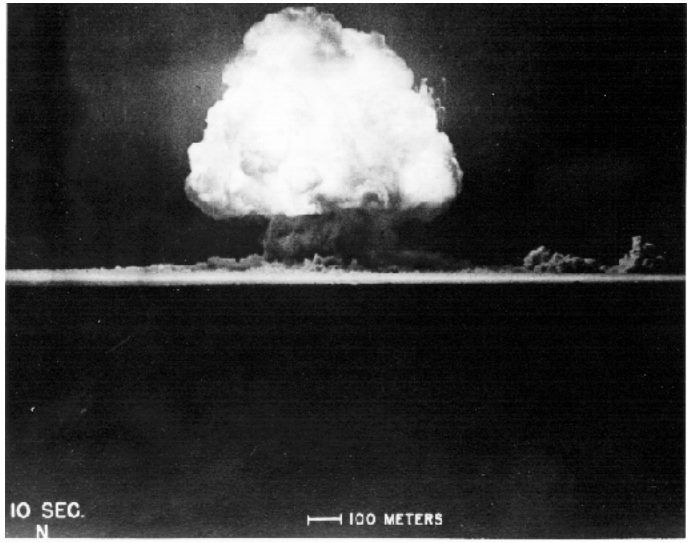
Keep *n* events, no more random number...

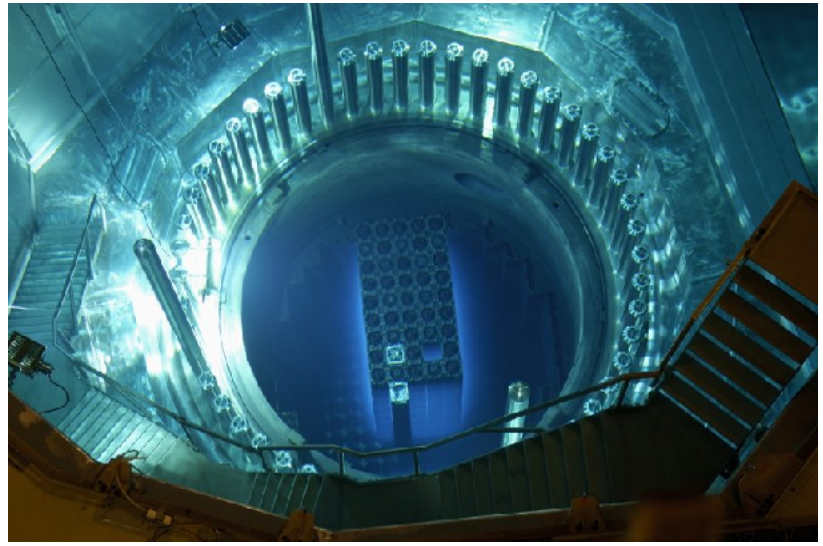
But associate a weight *p* to each of them (we set $\xi = p$)

Retain statistical accuracy ($1/\div n$)

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
- Does not to date handle crystalline / ordered material and coherent scattering of neutrons due to the focus on high energies





Examples of Monte Carlo programs

Each time physics takes place (scattering, absorption, …) random choices are made.

Light ray-tracing: PoV-RAY and others …

Nuclear reactor simulations (neutron transport):

MCNP, Tripoli, GEANT4, FLUKA

Neutron Ray-Tracing propagation:

***McStas <www.mcstas.org>**, Vitess, Restrax, NISP, IDEAS, McVine*

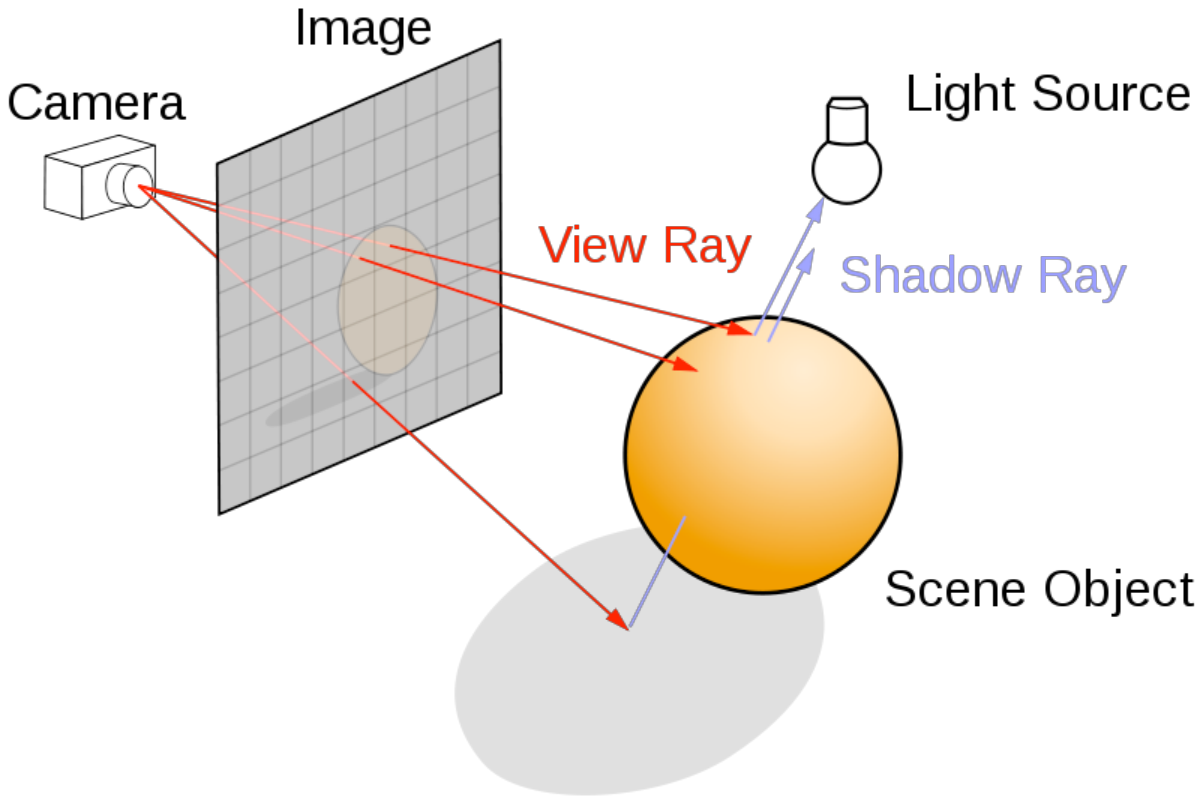
*Neutrons are described as **(r, v, s, t)**, and are transported along instrument models.*

Propagation simply uses Newton rules, incl. gravitation.

X-ray tracing

Shadow, McXtrace, RAY, …

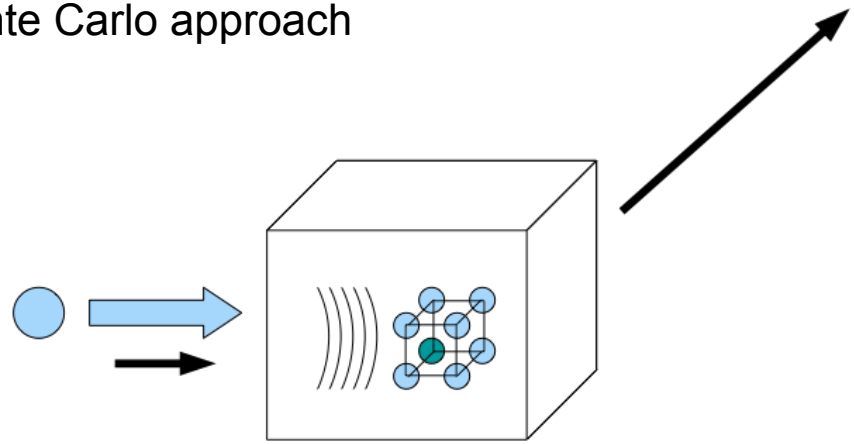
Ray-tracing methods



- When neutrons move in “free space”, we use ray-tracing - but in most cases in direction source -> detector
- Of course parabolas rather than straight lines are uses to implement gravity

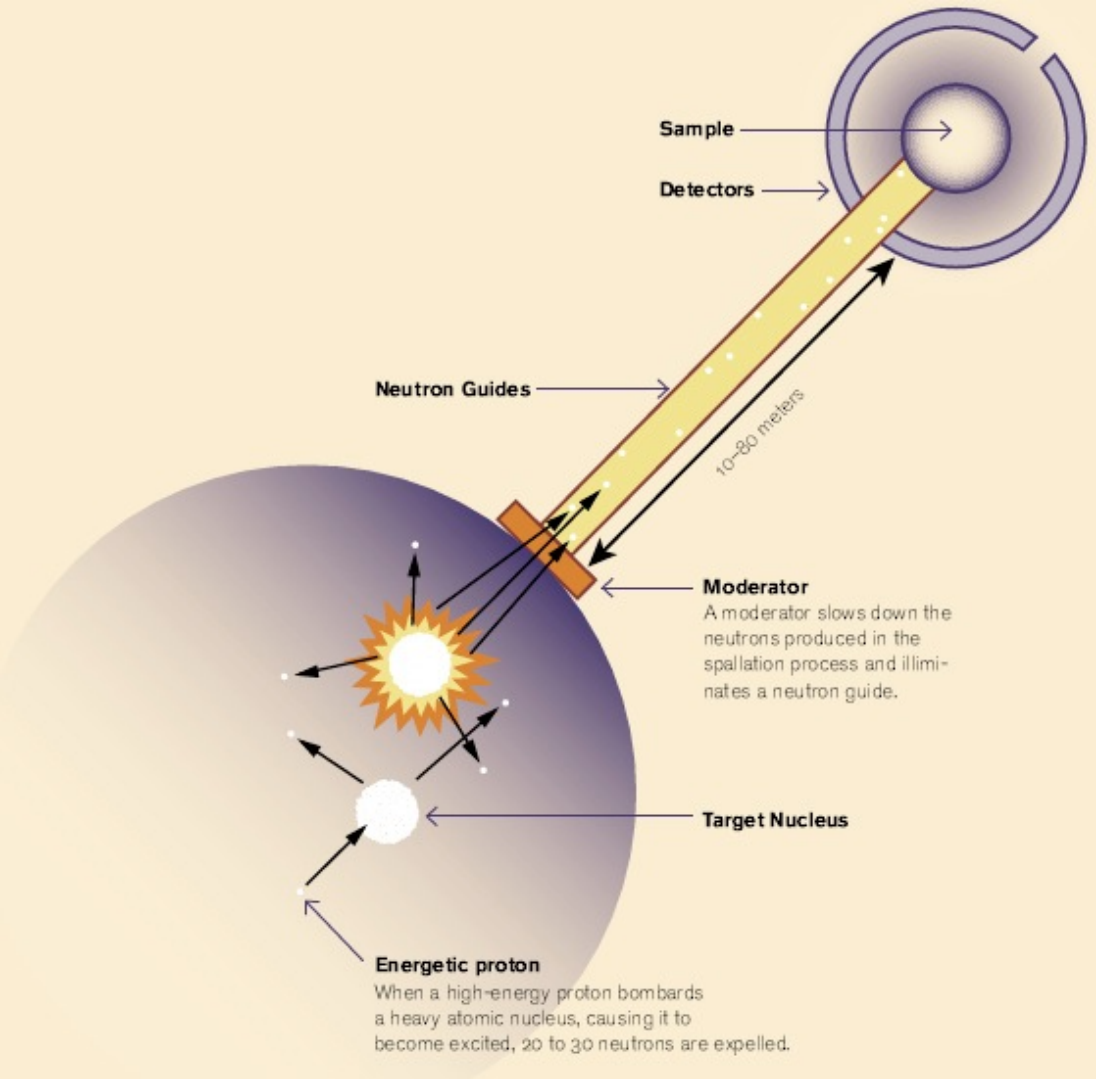
Elements of Monte-Carlo raytracing

- 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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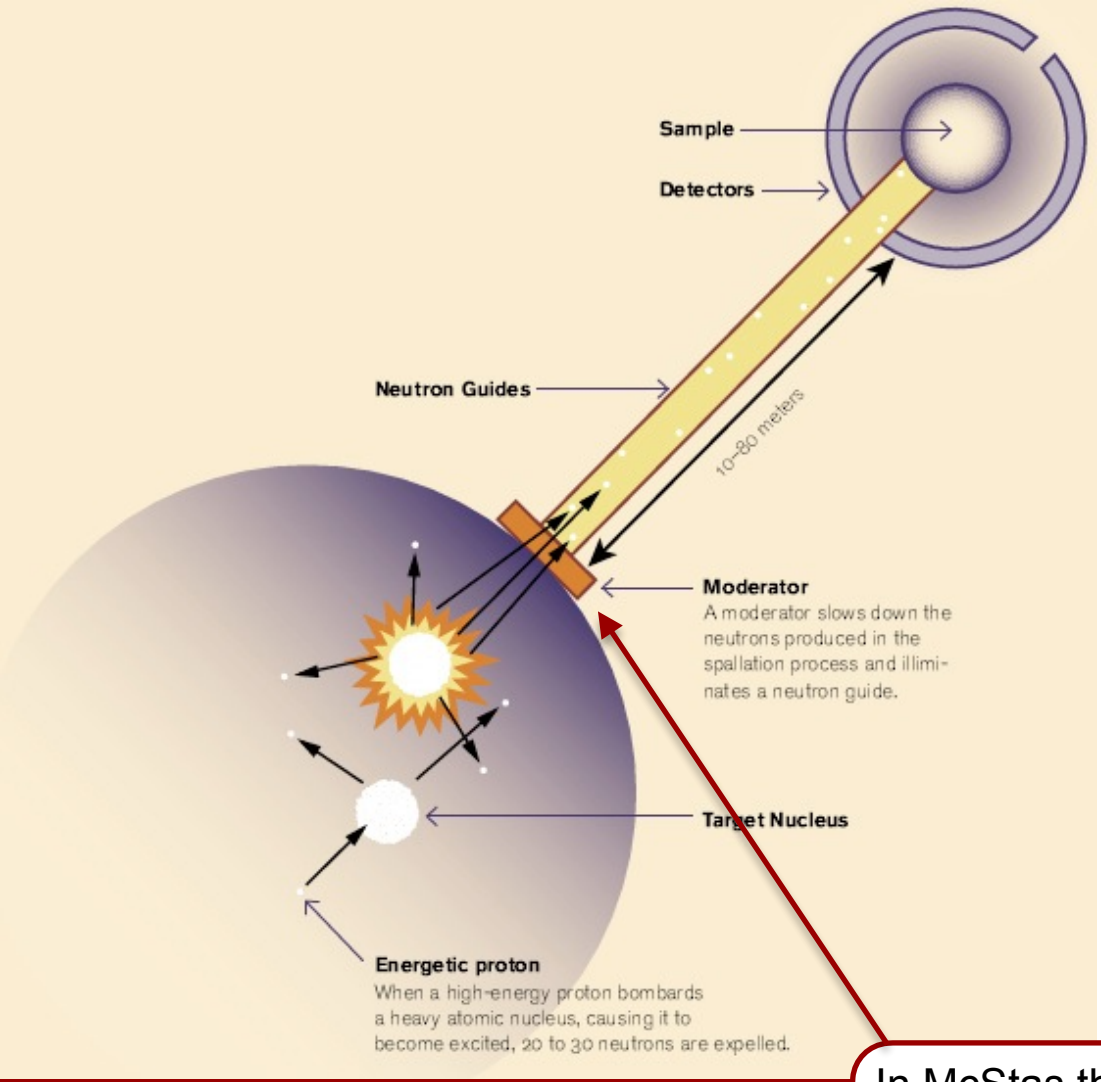

In McStas the moderator is the “source”

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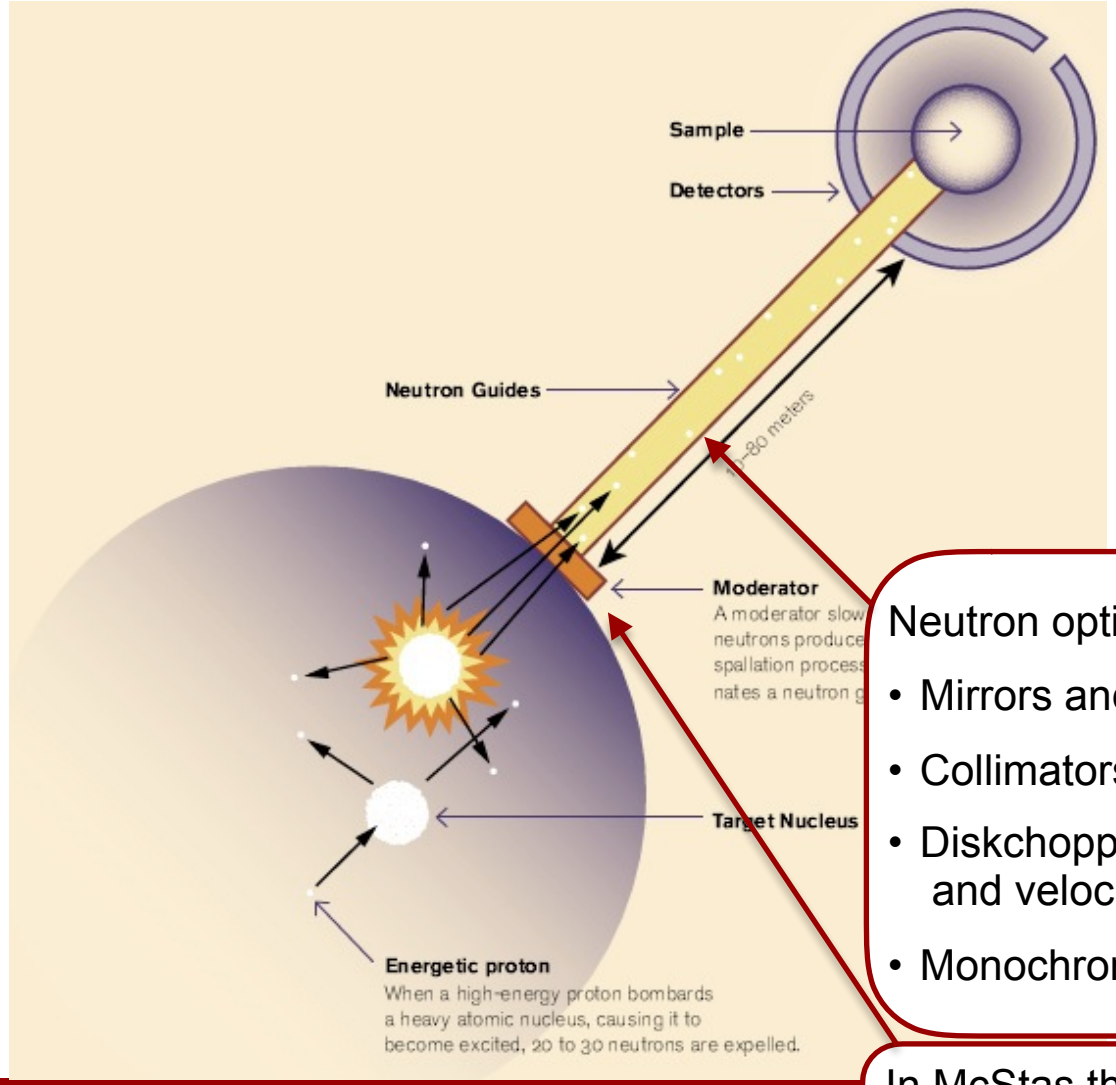
Components of neutron instruments



Neutron optics include things like:

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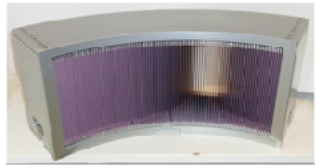
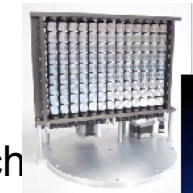
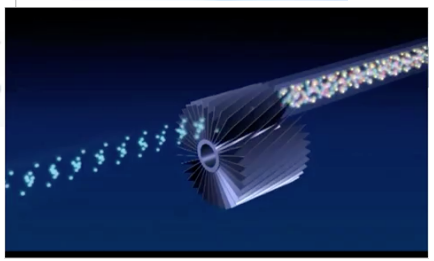
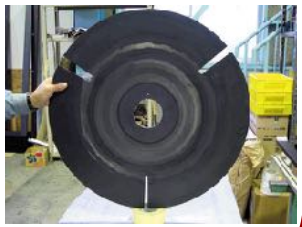
- Monochromators/Analysers

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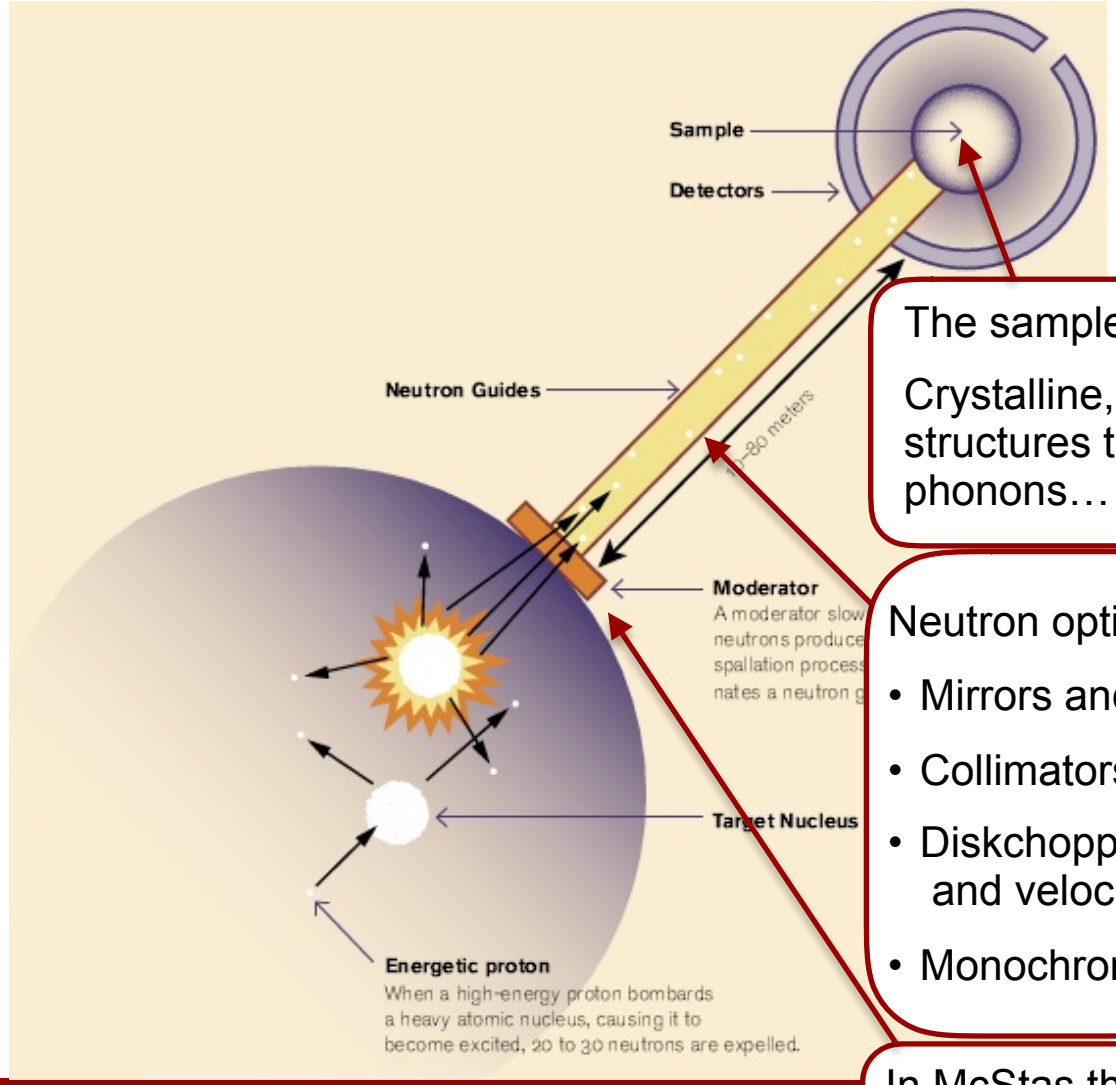
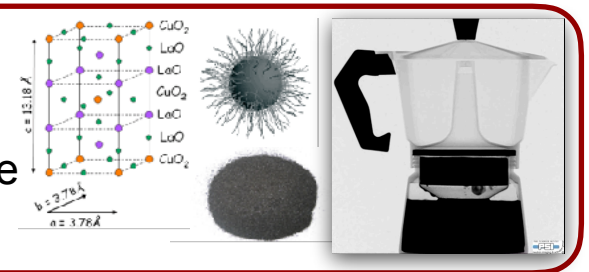


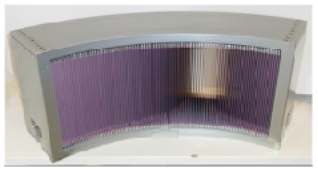
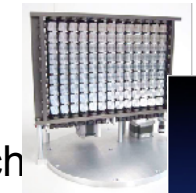
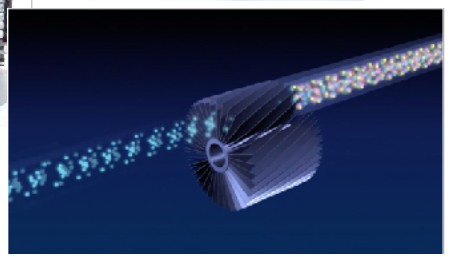
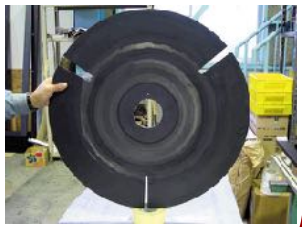
The sample:

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



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”

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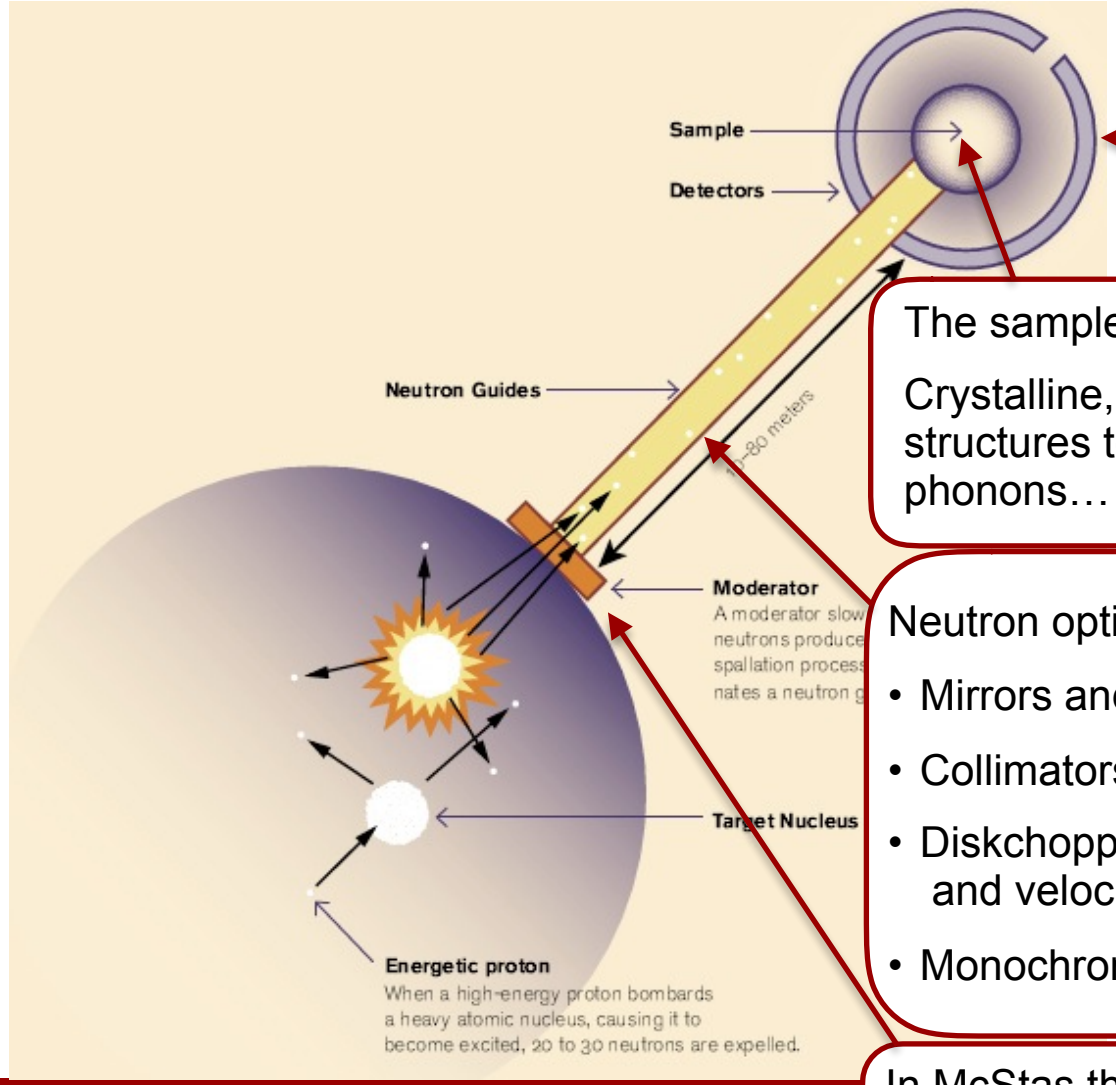
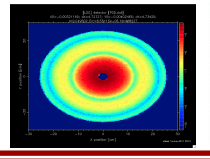
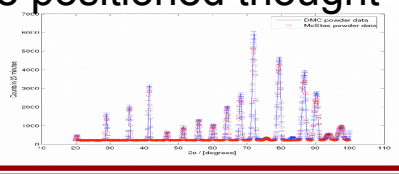
Components of neutron instruments



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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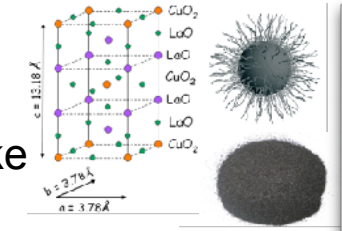

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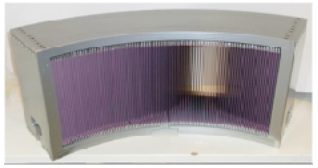

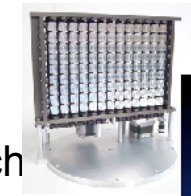

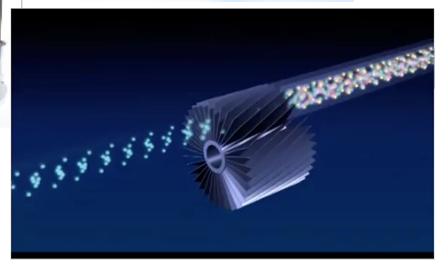

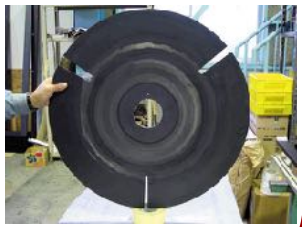

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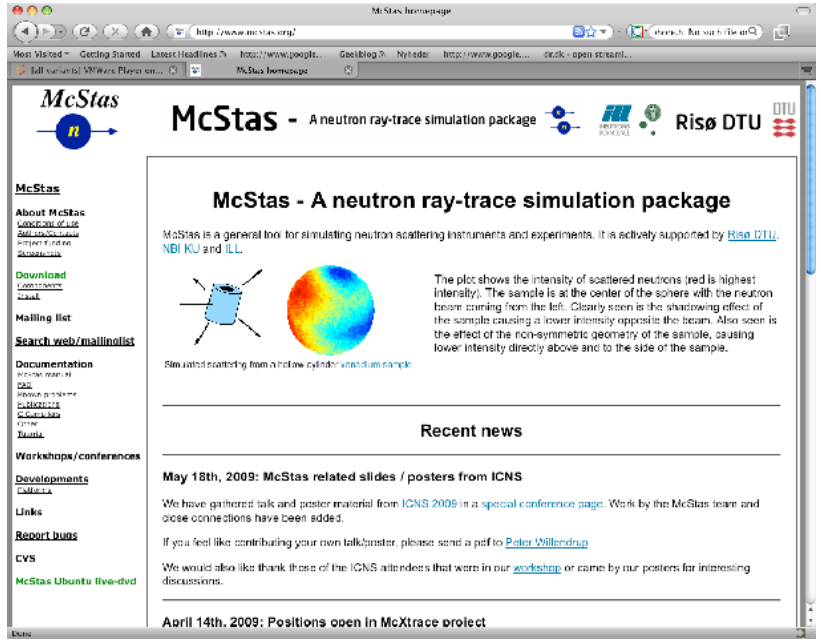
McStas Introduction

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

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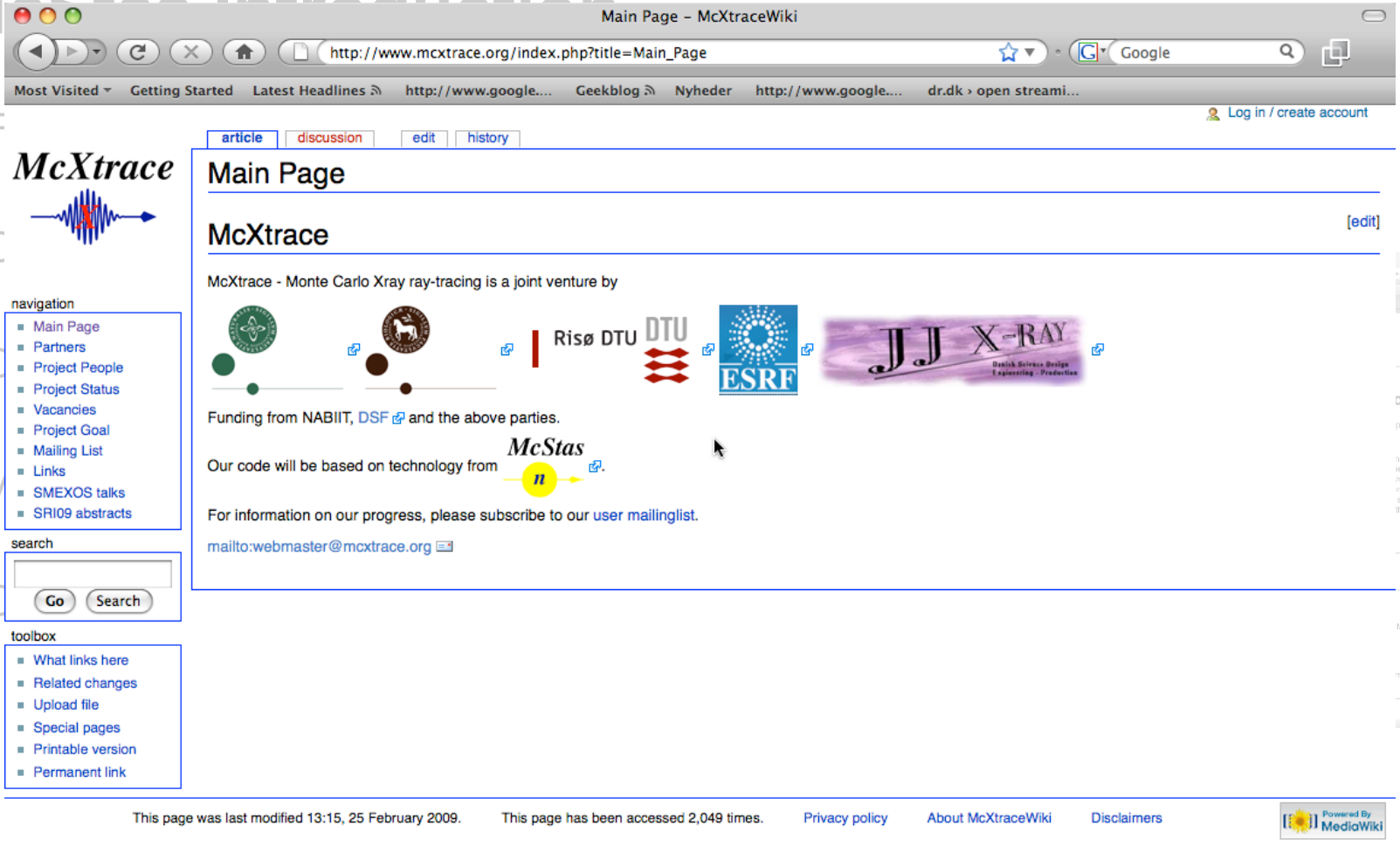
McXtrace - since jan 2009 similar for X-rays



- Synergy, knowledge transfer, shared infrastructure

Used in many places

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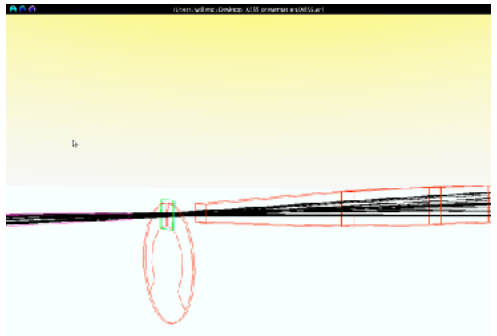
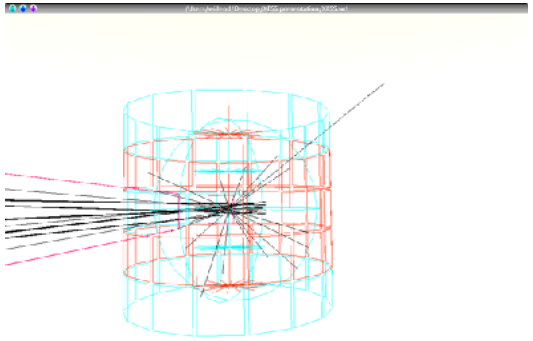
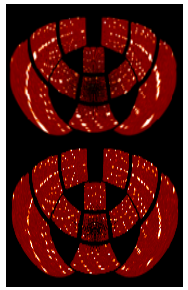
McStas

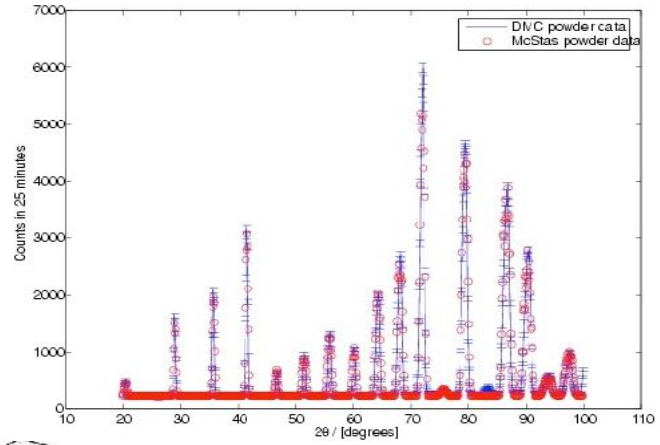
What is McStas used for?

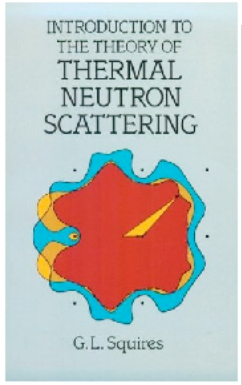
- Instrumentation
- Planning
- Construction
- Virtual experiments
- Data analysis
- Teaching
  (KU, DTU)

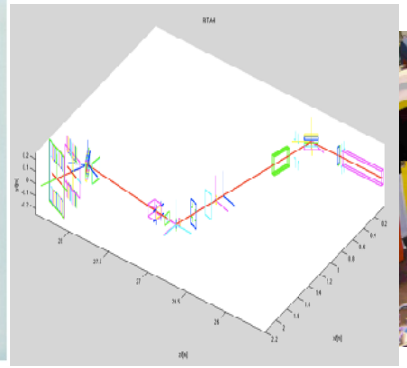


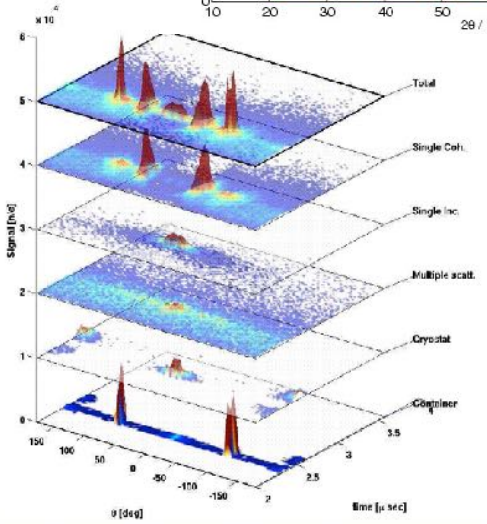












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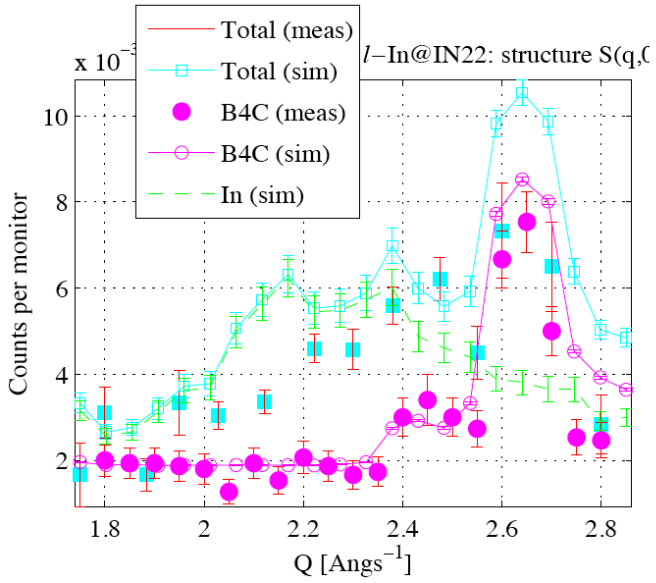
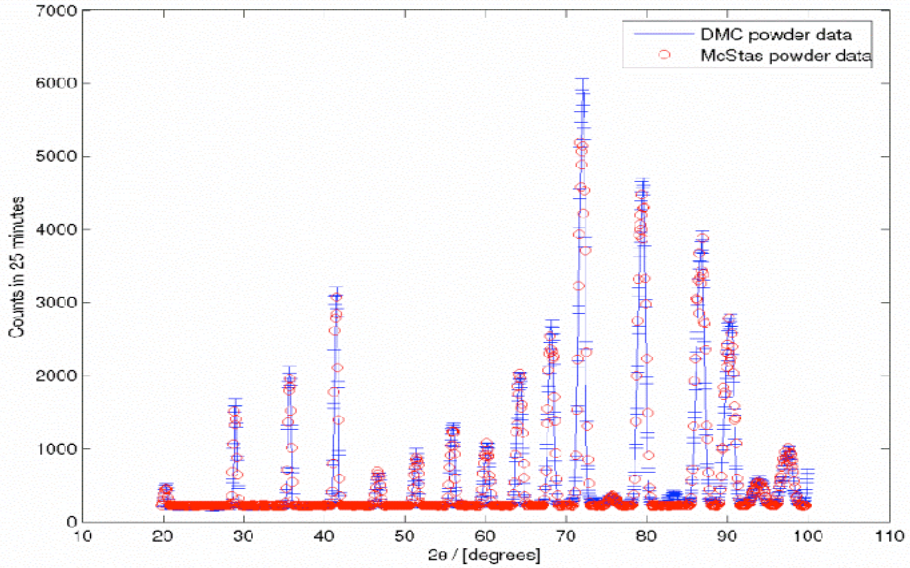
Reliability - cross comparisons

- 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.

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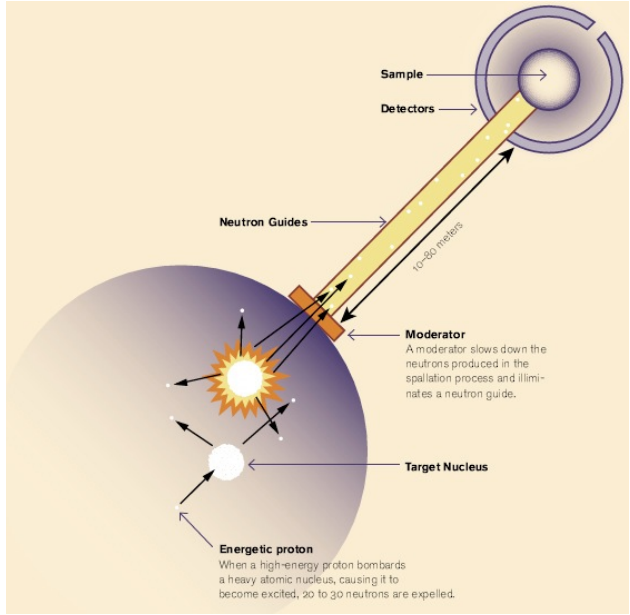
McStas overview

- 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.

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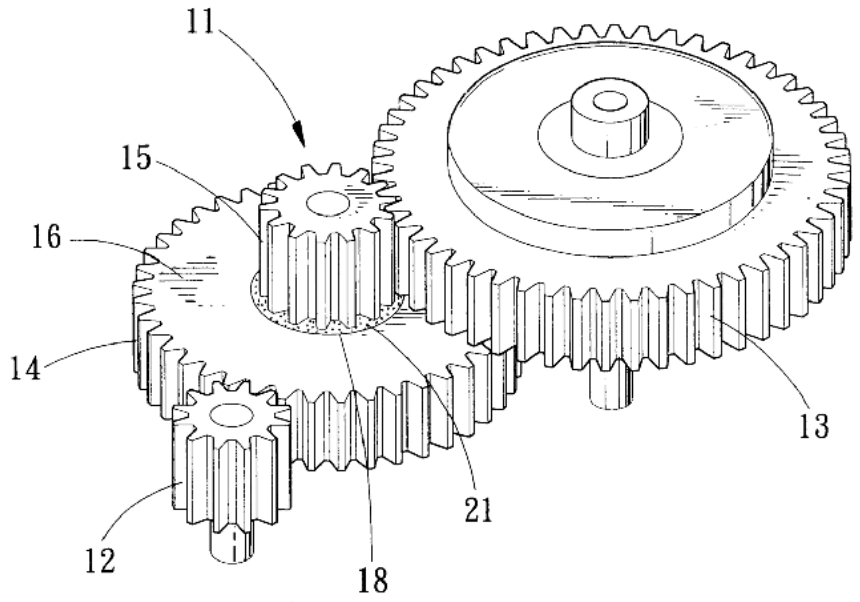
Under-the-hood / inner workings

- 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
  - ...



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Implementation

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

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!

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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

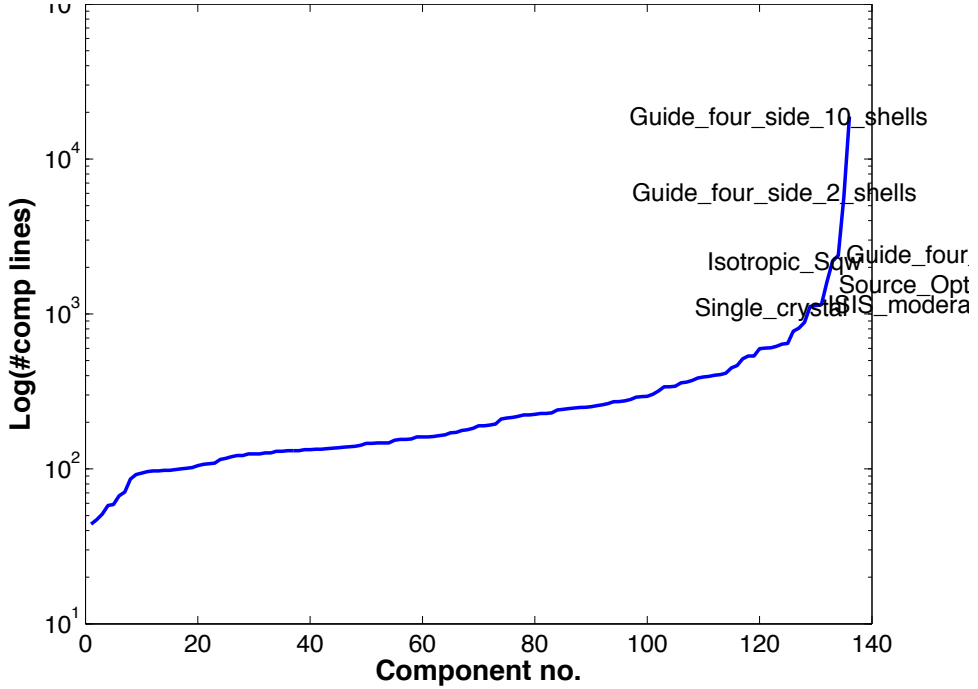
Output is a single c-file, which can be compiled using e.g. gcc.

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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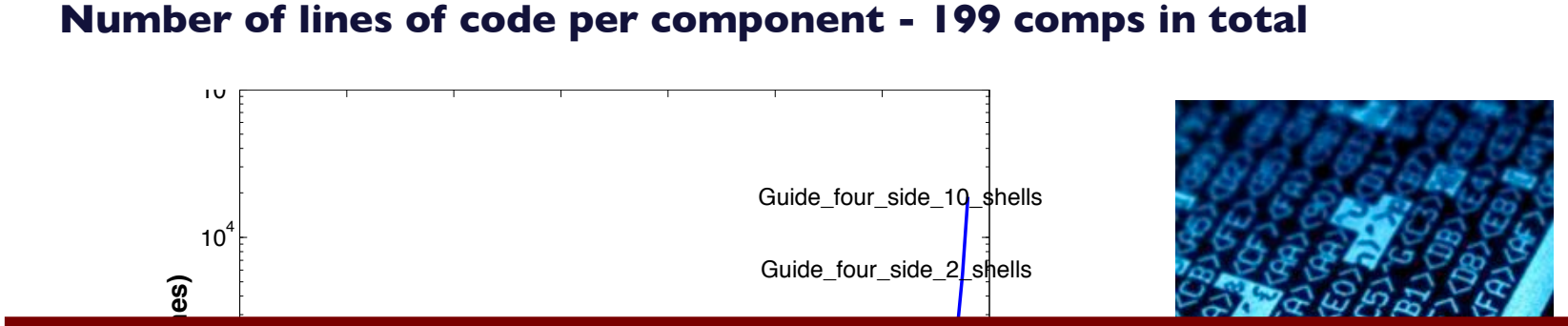
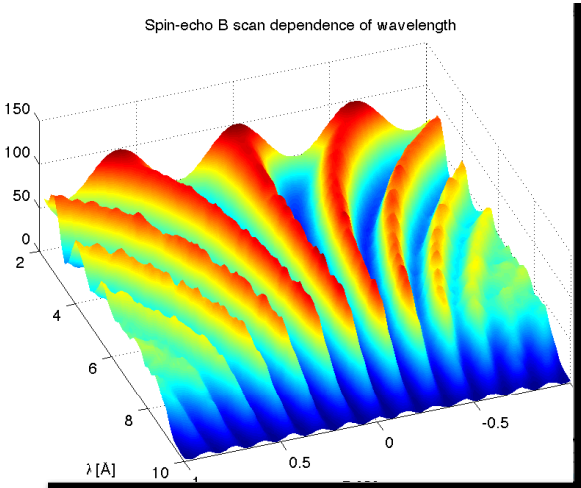
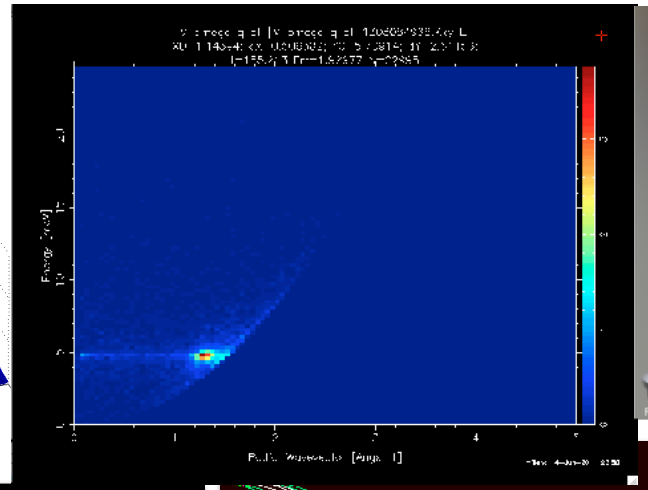
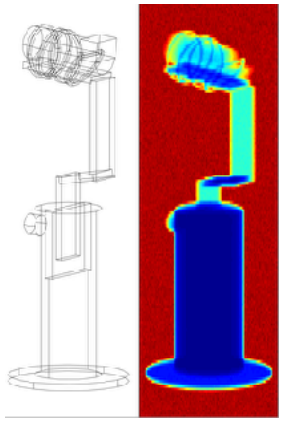


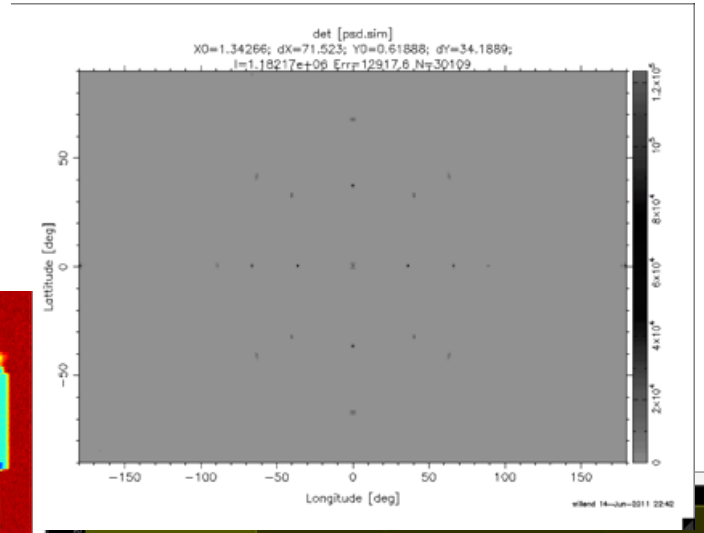
- Well-developed community support
  - –30-40% of existing and new additions are from users
  - –No direct refereeing of the code, but these requirements:
    - –At least one test-instrument
    - –Meaningful documentation headers (in-code docs)
  - –Contributions go in dedicated contrib/ section of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

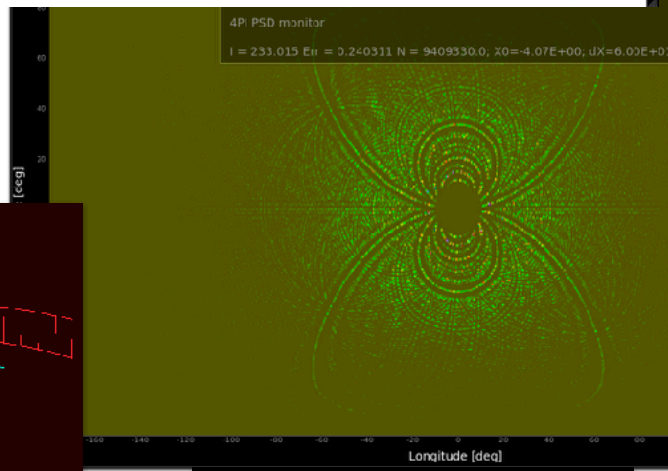
Example suite: ~140 instruments

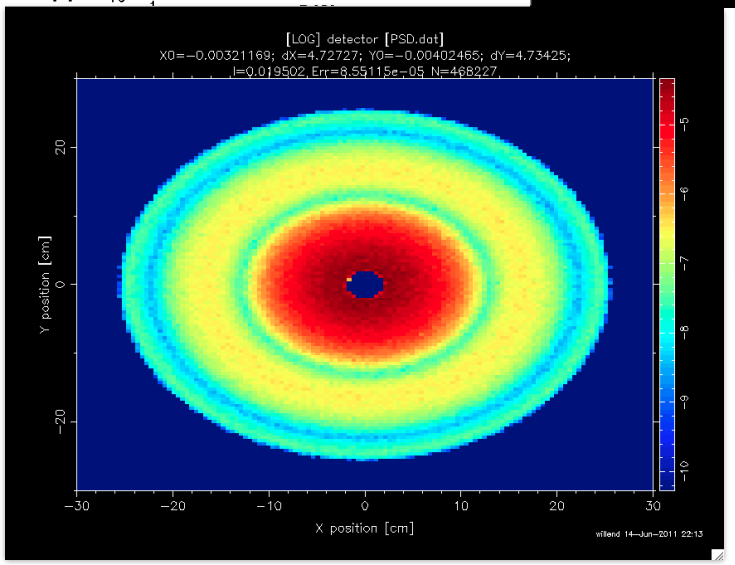


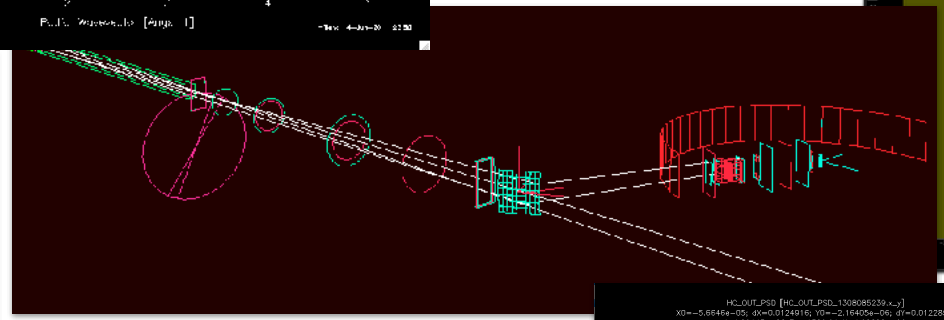


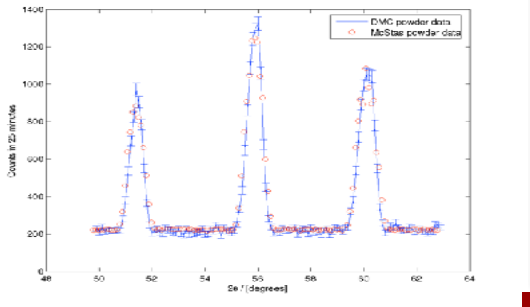


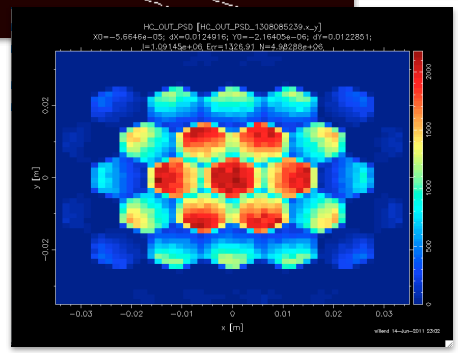


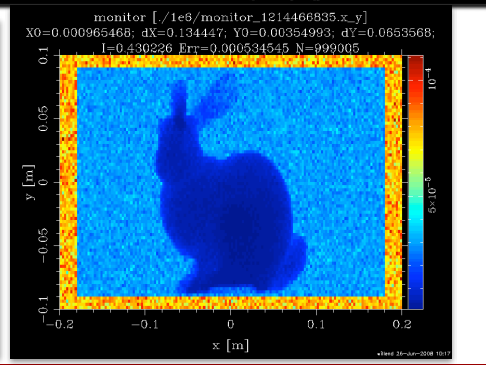












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DTU

ESS EUROPEAN SPALLATION SOURCE

CSNS

中国散裂中子源

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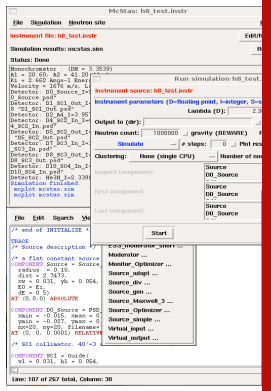
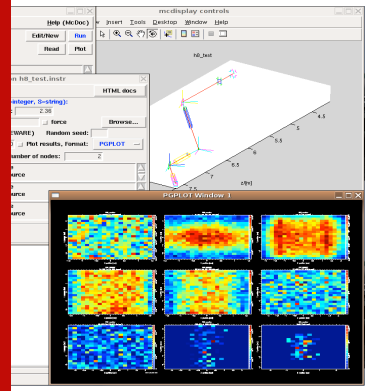
McStas

DTU PSI NEUTRONS FOR SCIENCE ESS EUROPEAN SPALLATION SOURCE





THIS IS NOT THE END

IT'S JUST

THE BEGINNING