McStas Introduction

Science & Technology Facilities Council
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ISIS STFC McStas training April 26th-28th 2017

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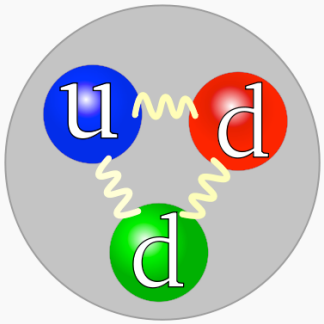
Agenda

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

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, 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

Subatomic particle discovered by Sir James Chadwick, 1932

The Neutron

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

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

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

Mr. Neutron

	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

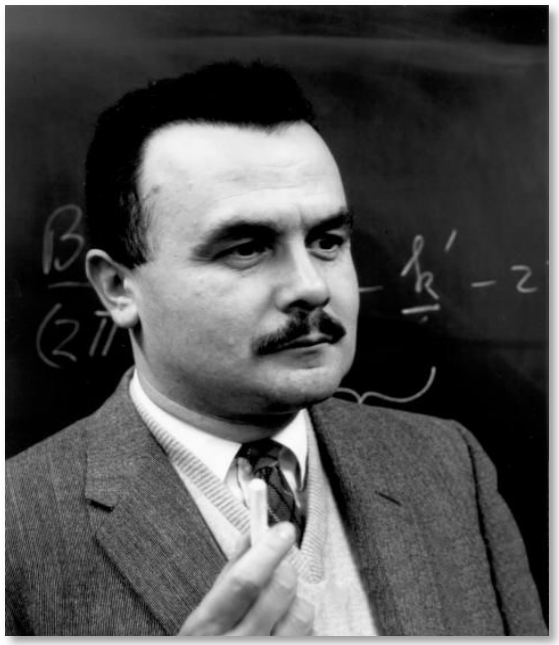
Cross section: coherent + incoherent + absorption

DTU ESS EUROPEAN SPALLATION SOURCE

Nobel Prize in Physics, 1994

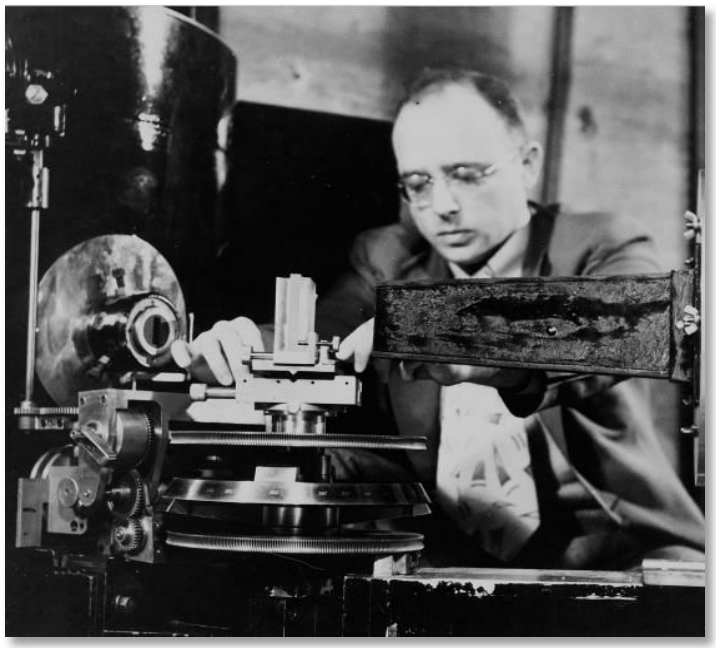
Awarded for “pioneering contributions to the development of neutron scattering techniques for studies of condensed matter”

Bertram N. Brockhouse



Neutron spectroscopy

Clifford G. Shull



Neutron diffraction technique

1994 Nobel prize to Shull & Brockhouse

Neutrons show where the atoms are….

When the neutrons collide with atoms in the sample material, they change direction (are scattered) – elastic scattering.

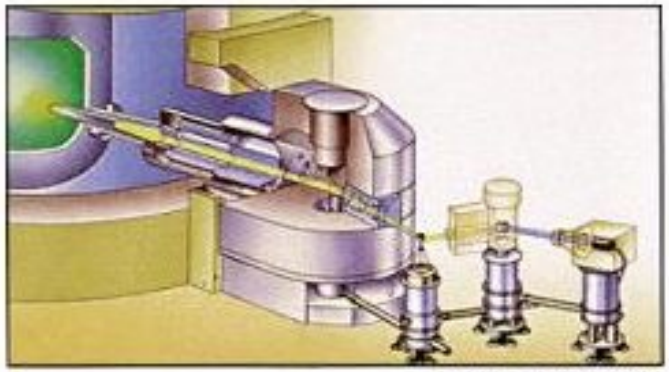
Atoms in a crystalline sample

Research reactor

Neutron beam

Detectors record the directions of the neutrons and a diffraction pattern is obtained.
The pattern shows the positions of the atoms relative to one another.

Crystal that sorts and forwards neutrons of a certain wavelength (energy) – mono-chromatized neutrons



3-axis spectrometer

…and what the atoms do.

3-axis spectrometer with rotatable crystals and rotatable sample

Atoms in a crystalline sample

Changes in the energy of the neutrons are first analysed in an analyser crystal...

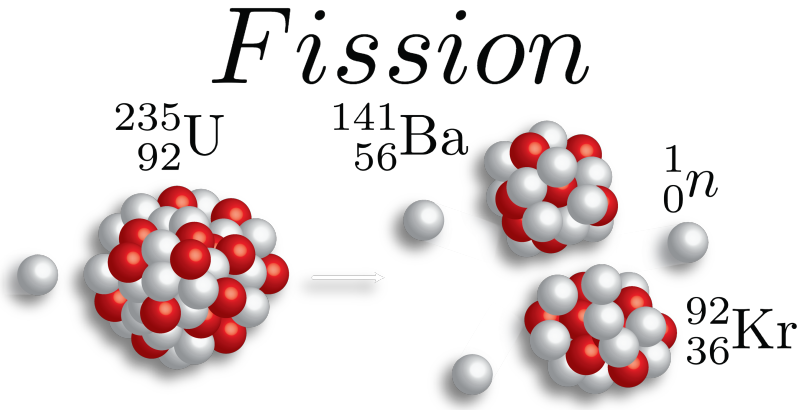
Neutron beam

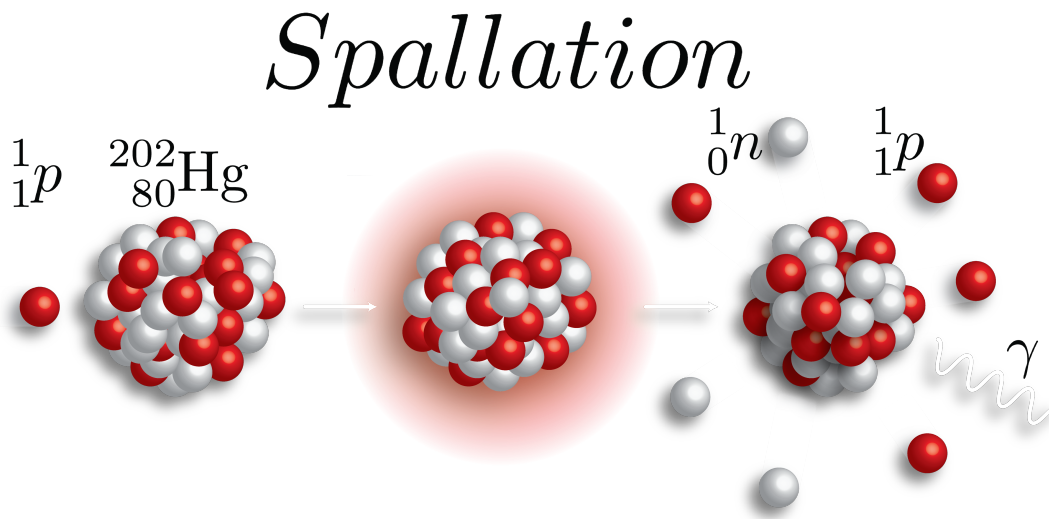
When the neutrons penetrate the sample they start or cancel oscillations in the atoms. If the neutrons create phonons or magnons they themselves lose the energy these absorb – inelastic scattering

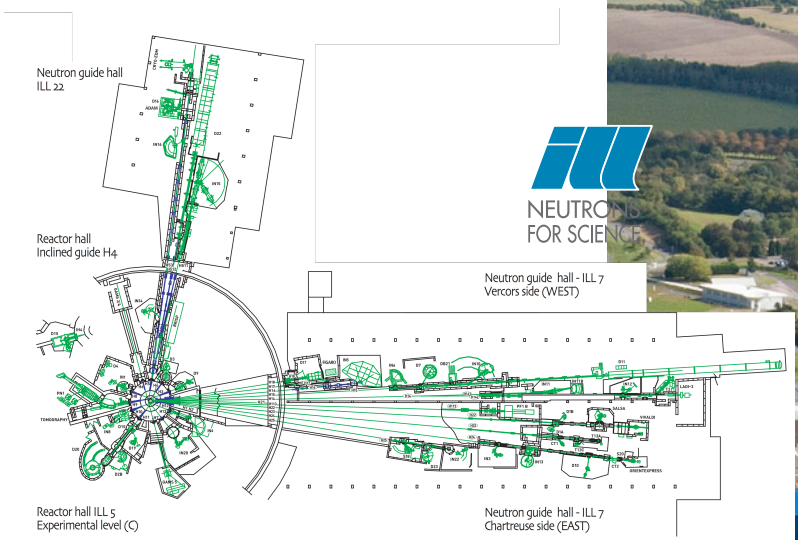
Crystal that sorts and forwards neutrons of a certain wavelength (energy) – mono-chromatized neutrons

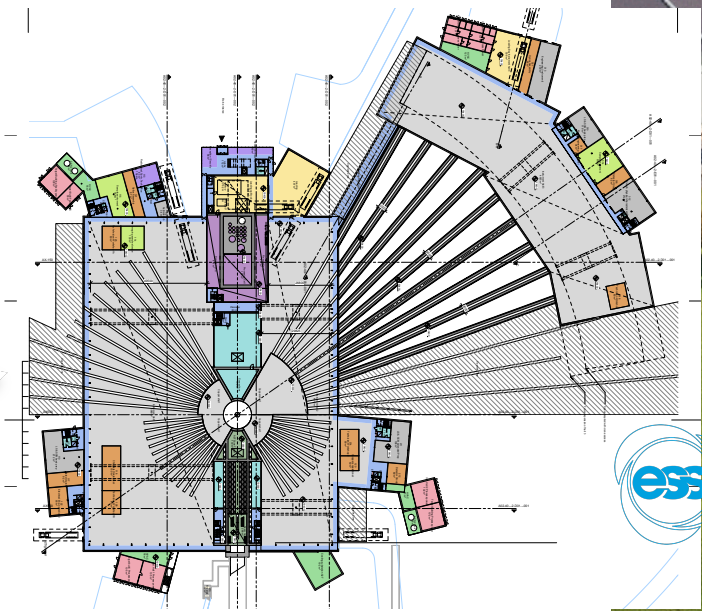
...and the neutrons then counted in a detector.

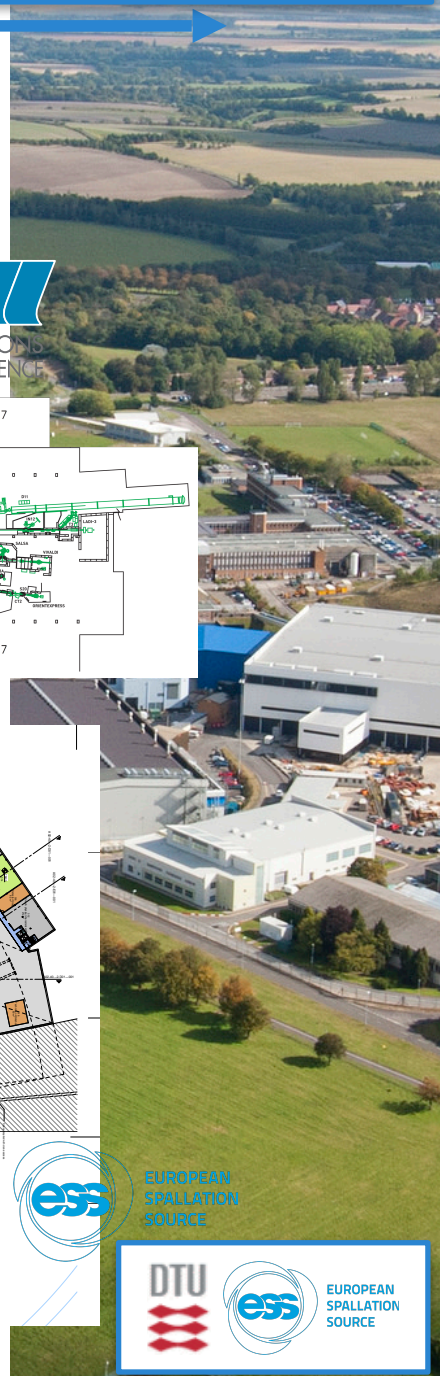
Neutron facilities











Origin of Monte Carlo methods

Used by Nature since ... (a long time) : diversity of Life

First application using computers:

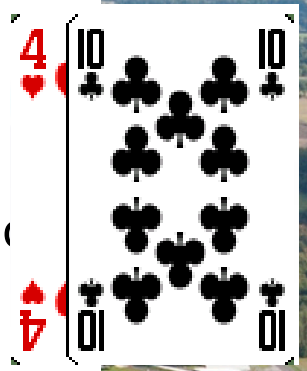
Metropolis, Ulam and Von Neumann at Los Alamos, 1943

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

Name:

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

What are Monte Carlo methods?



- Use random generators (play poker)
- Explore a complex and large phase space (many parameters)
- Integrates microscopic random events into measurable quantities n usual regular sampling integration

- Metropolis algorithm: model energy gap E as a probability

$$\lim_{n\to\infty} \frac{1}{n} \sum_{i=1, a<u_i<b}^{n} f(u_i) = \frac{1}{b-a} \int_a^b f(u)\,du$$

- Integrals converge faster than any other method (for d > 3) when using enough independent events (central limit theorem)

$$p \;\alpha\; e^{-E/kT}$$

- F. James, Rep. Prog. Phys., Vol. 43 (1980) 1145.

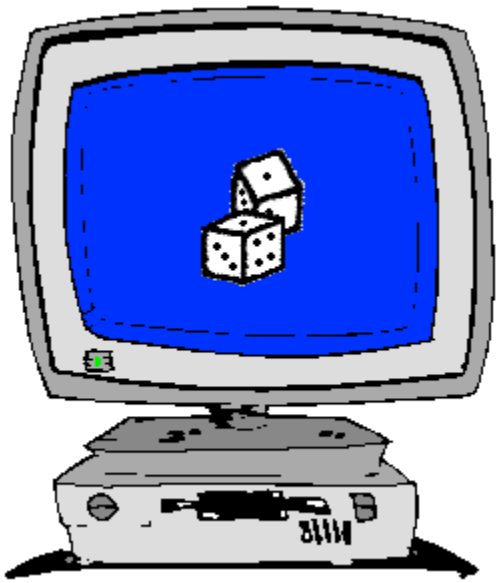
How to implement Monte Carlo methods ?

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 ($1/\div n$)

When to use Monte Carlo methods

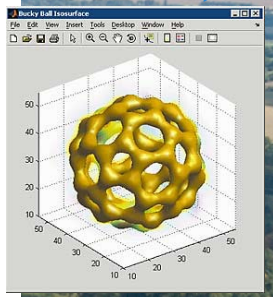
Dimensionality of phase space must be large (d > 5)

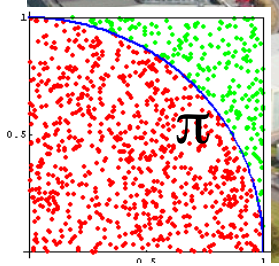
Overall complexity is beyond reasonable analytical methods

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 → π/4

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

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

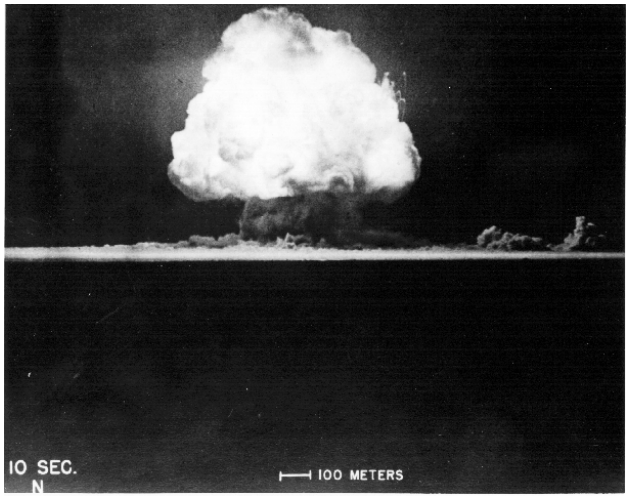
Propagation simply uses Newton rules, incl. gravitation.

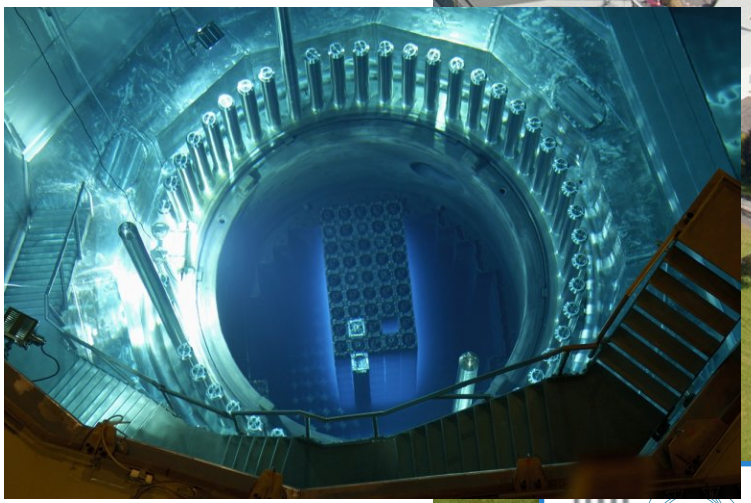
X-ray tracing

Shadow, McXtrace, RAY, …

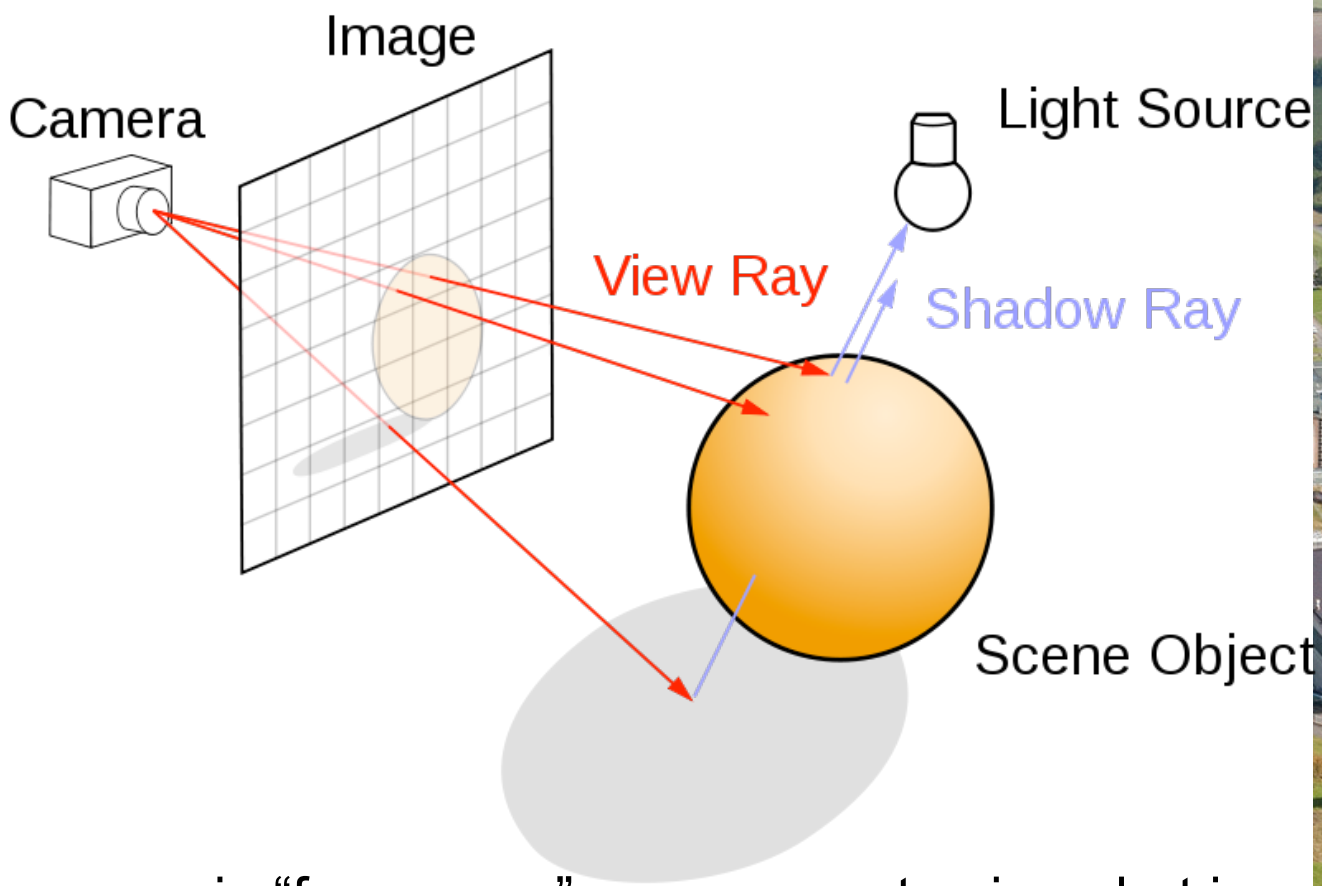
Monte Carlo techniques

- 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 MCNPX (or soon the merged MCNP6 code) 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 coherent scattering of neutrons due to the focus on high energies





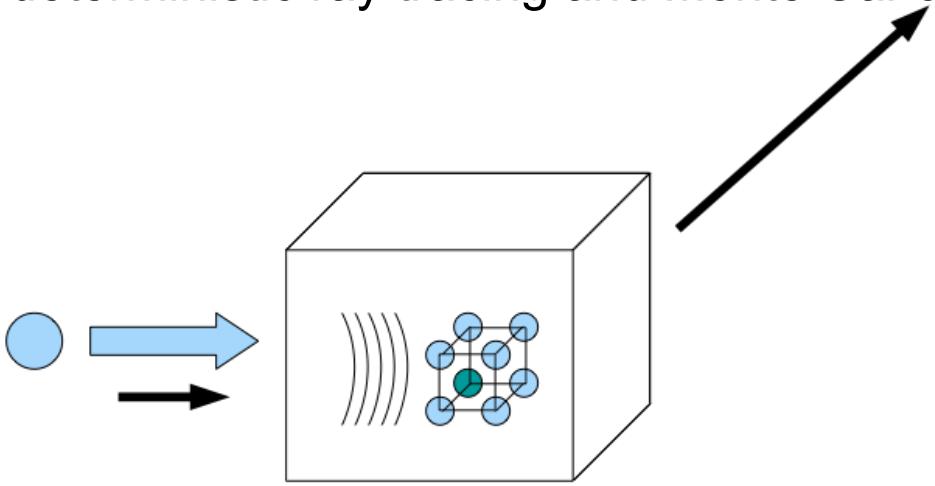
Ray-tracing methods



- 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

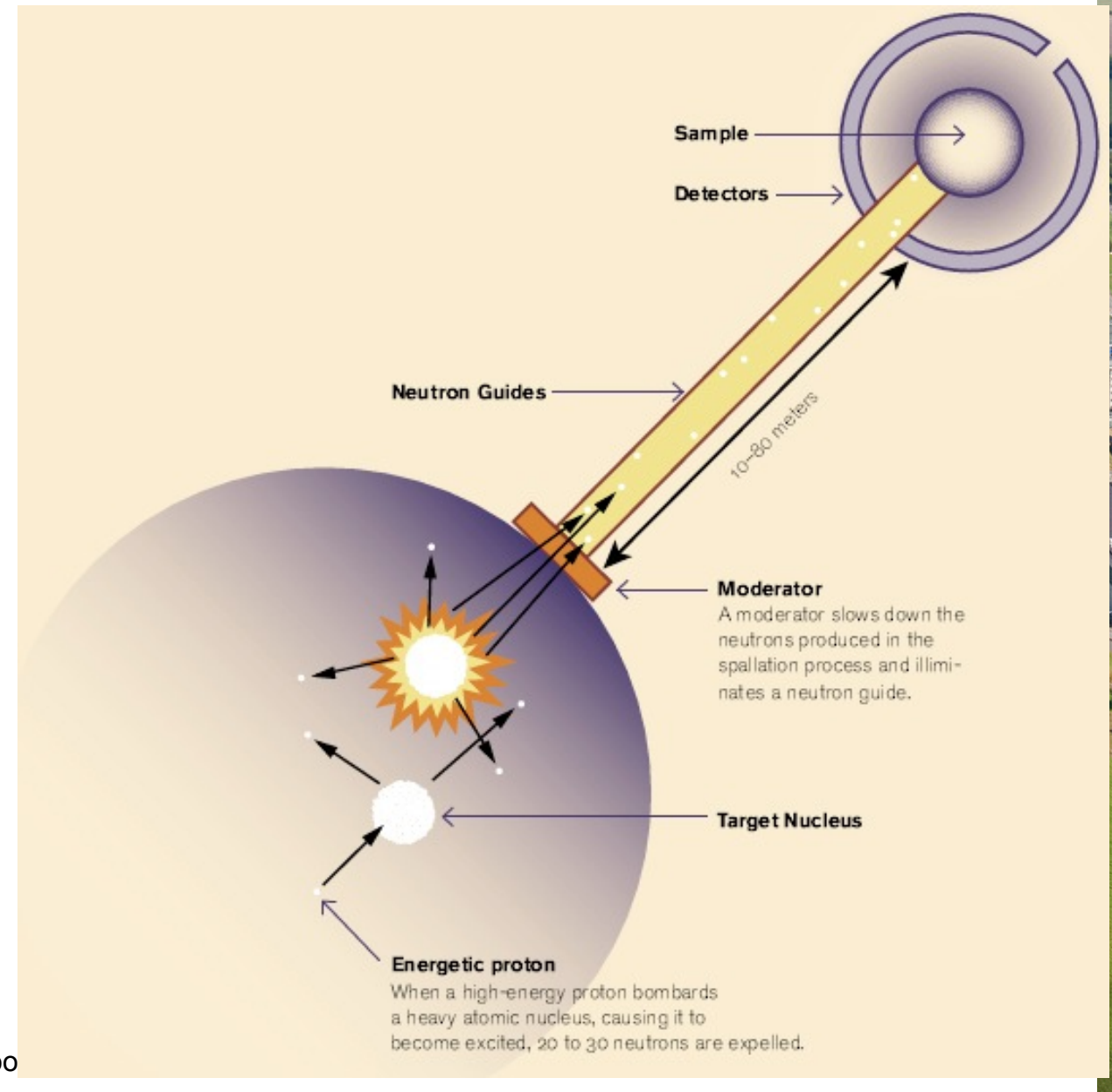
Elements of Monte-Carlo raytracing

- 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

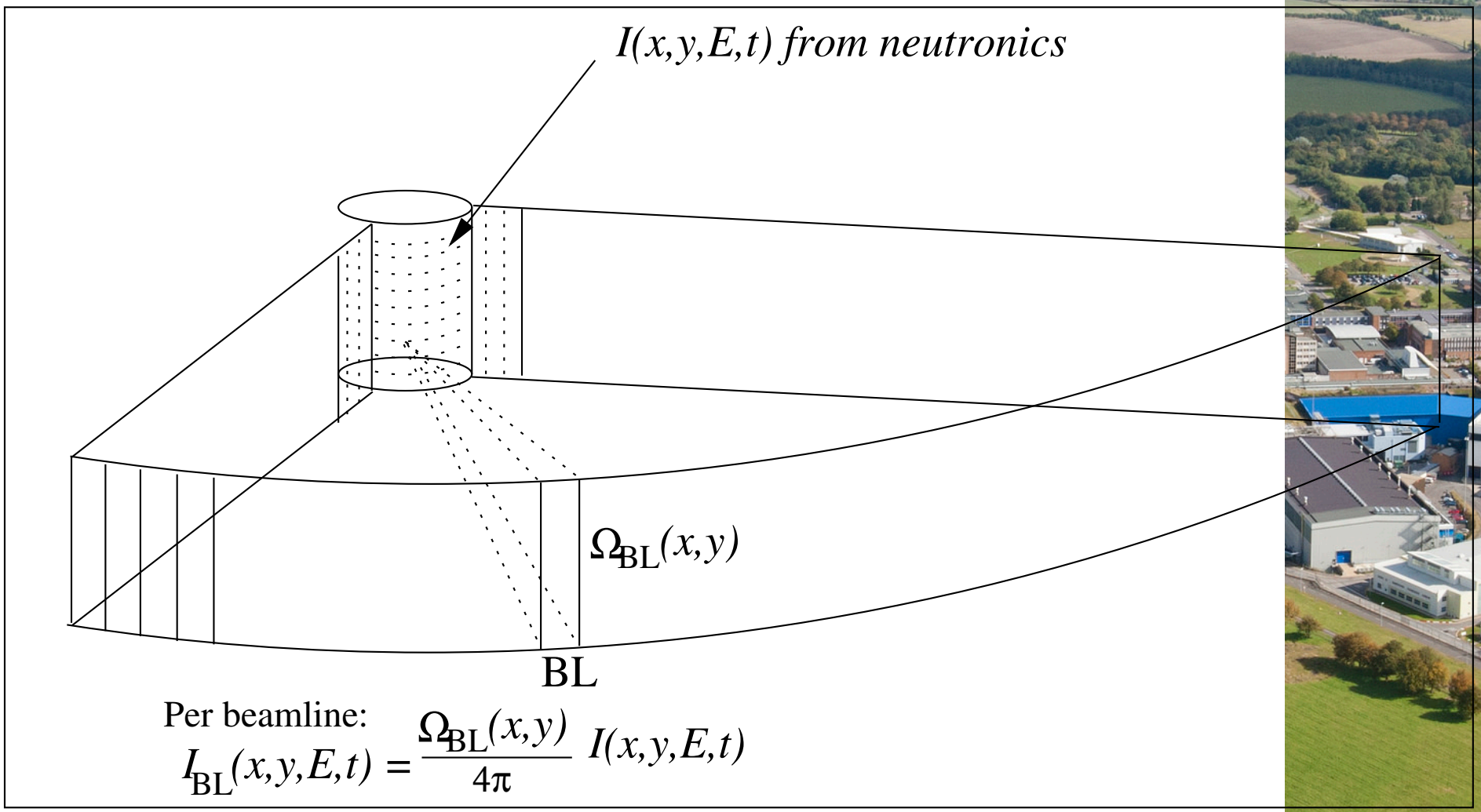


- Result: A realistic and efficient transport of neutrons in the thermal and cold range

Components of neutron instruments



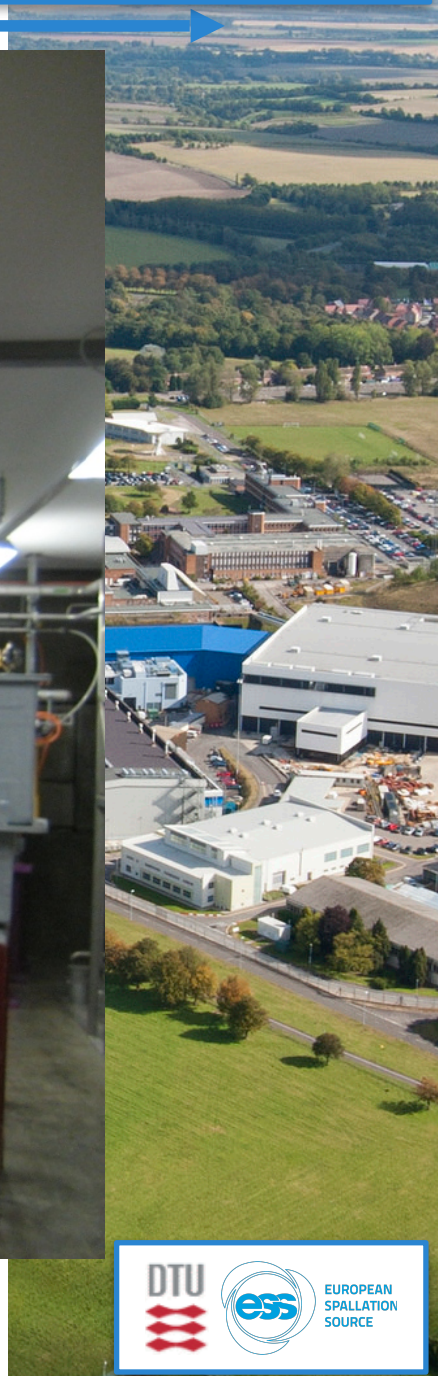
Moderators... (Where McStas starts)



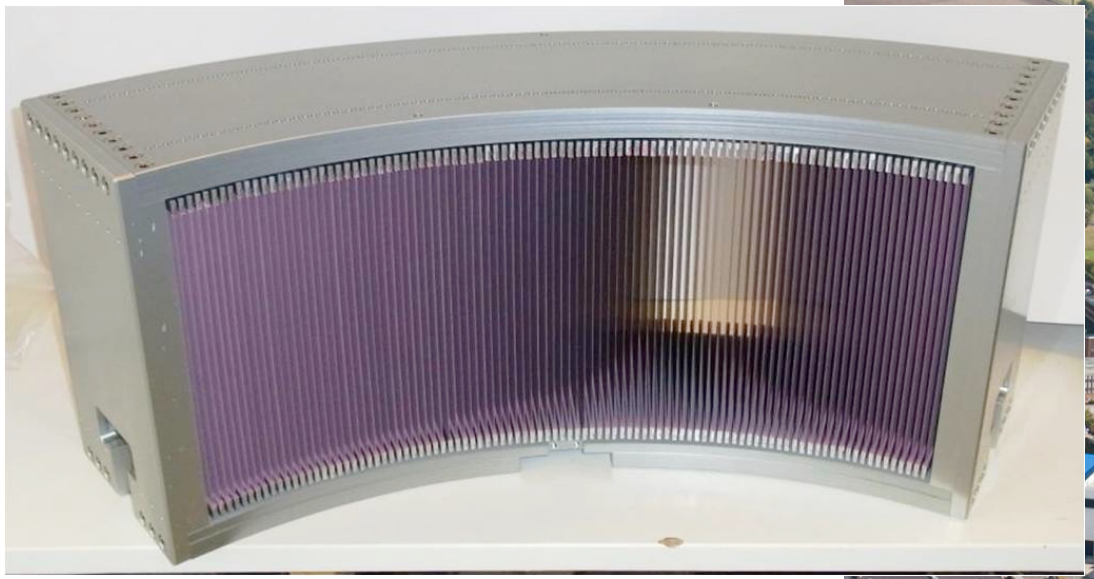
Per beamline:

$$I_{BL}(x,y,E,t) = \frac{\Omega_{BL}(x,y)}{4\pi} I(x,y,E,t)$$

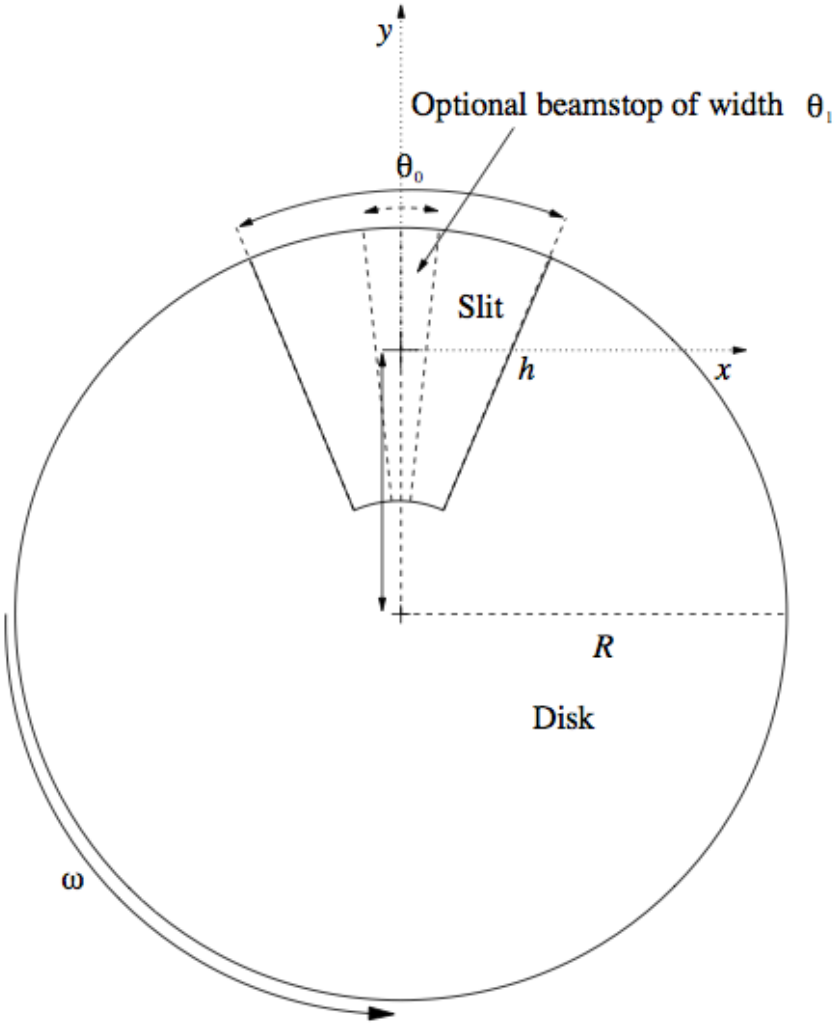
Neutron guides

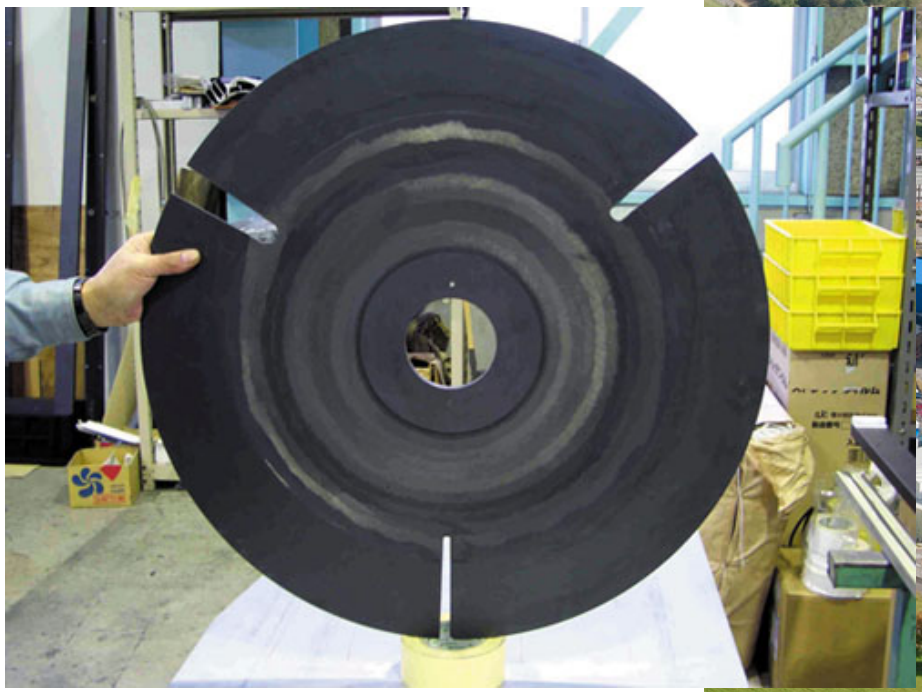


Collimators & slits



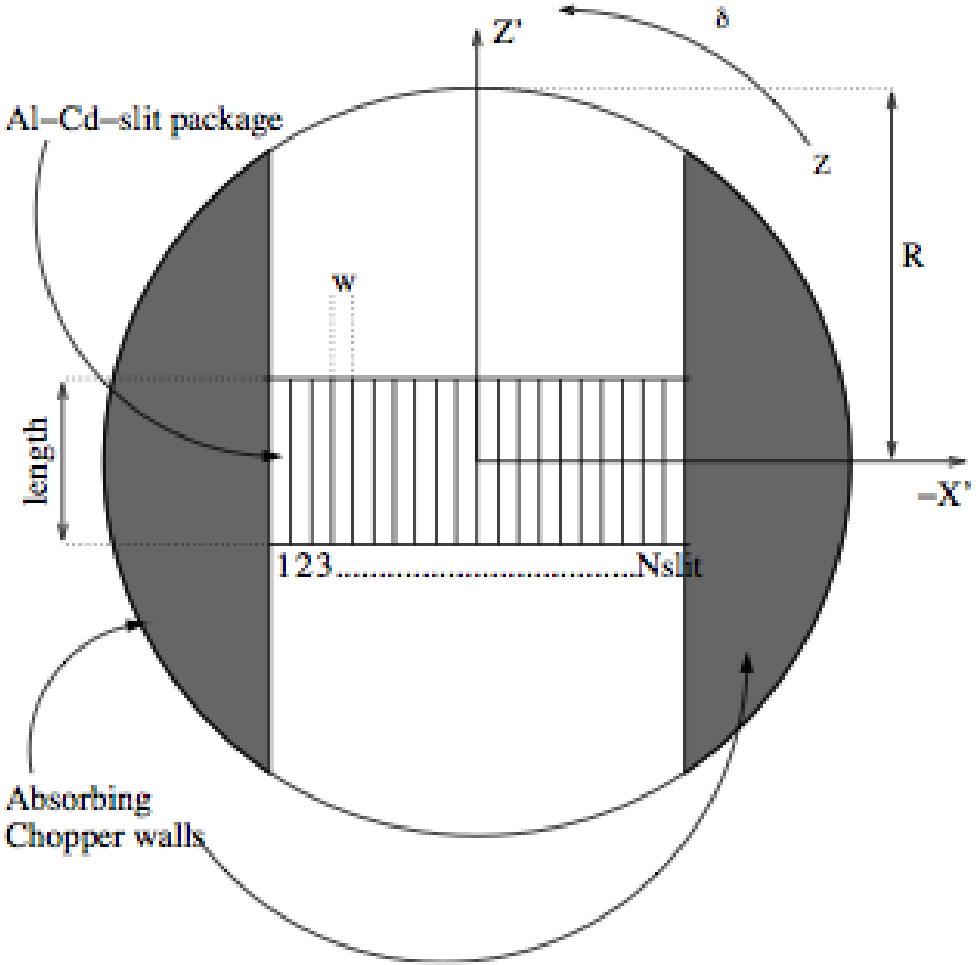
Disk Choppers

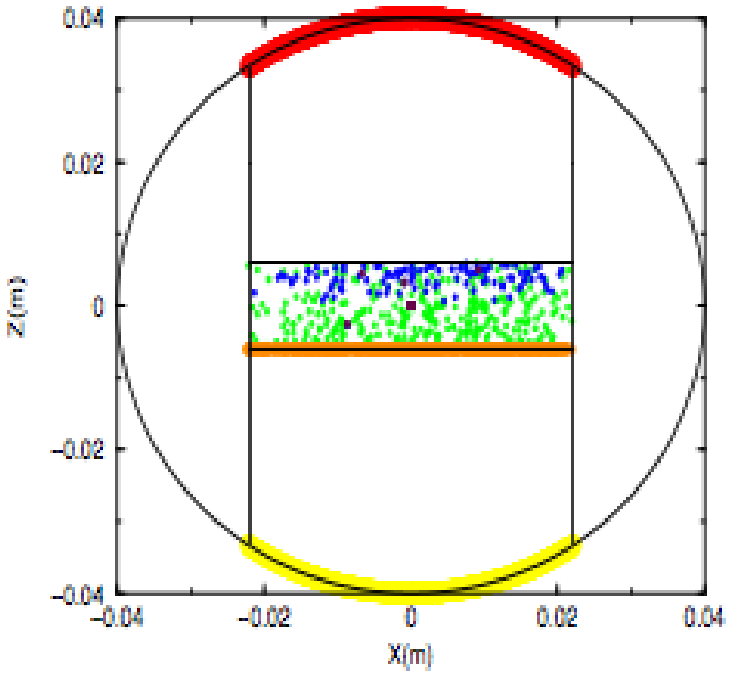




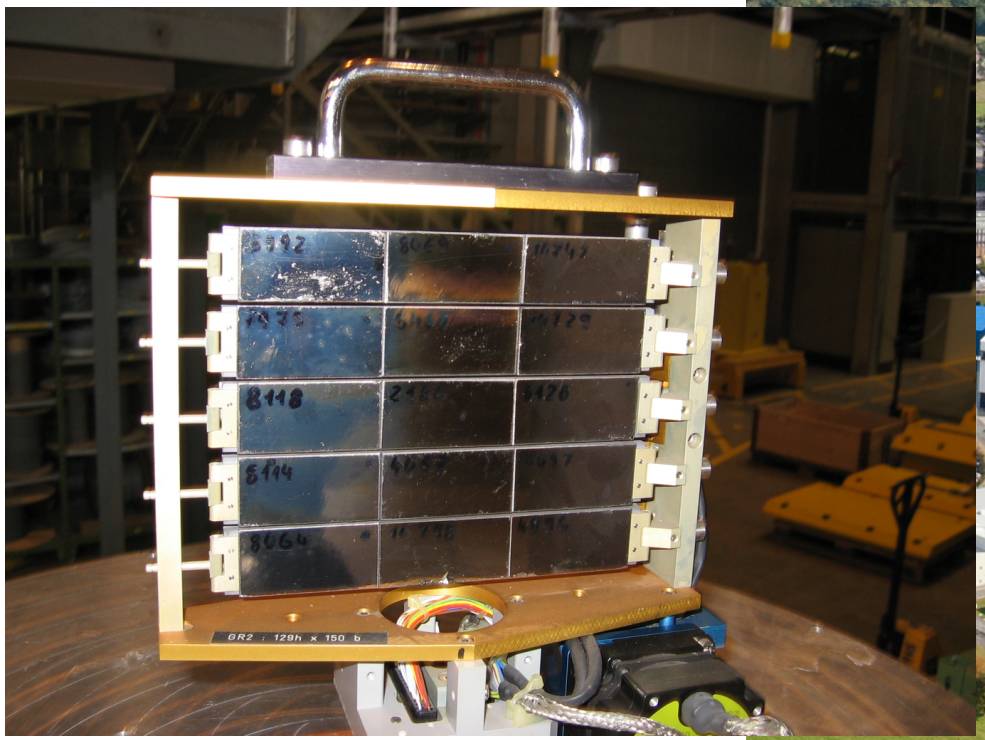
Velocity selector

Fermi Choppers

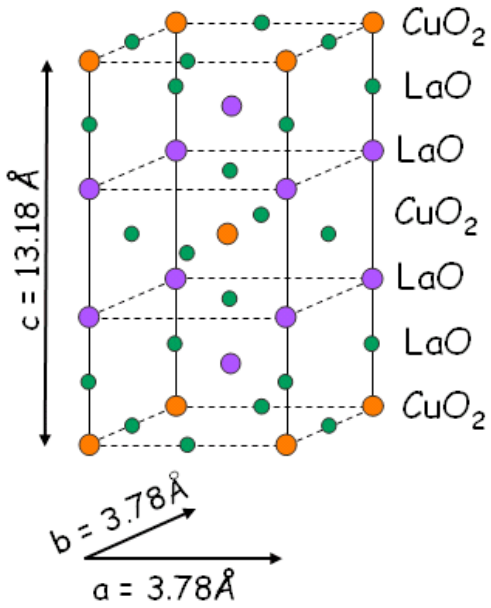


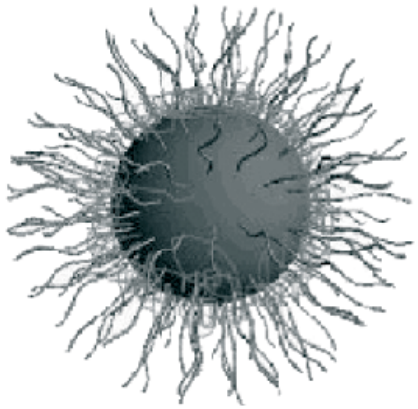


Crystal monochromators (and analyzers)



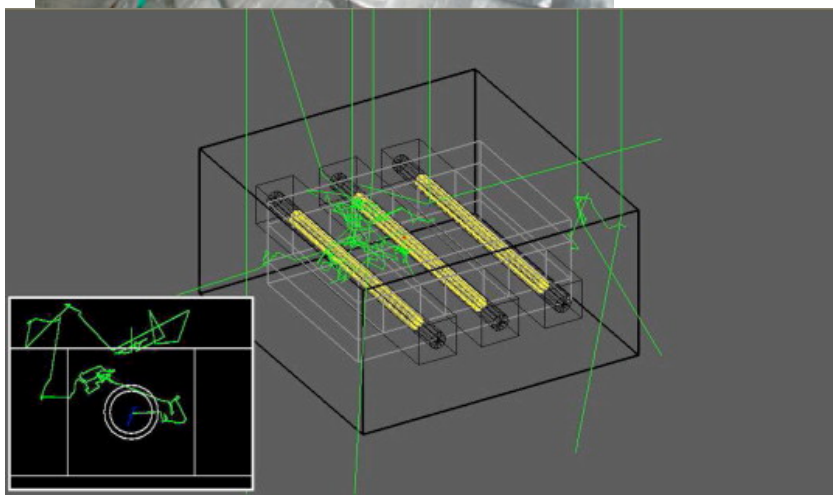
Samples studied...





Detectors

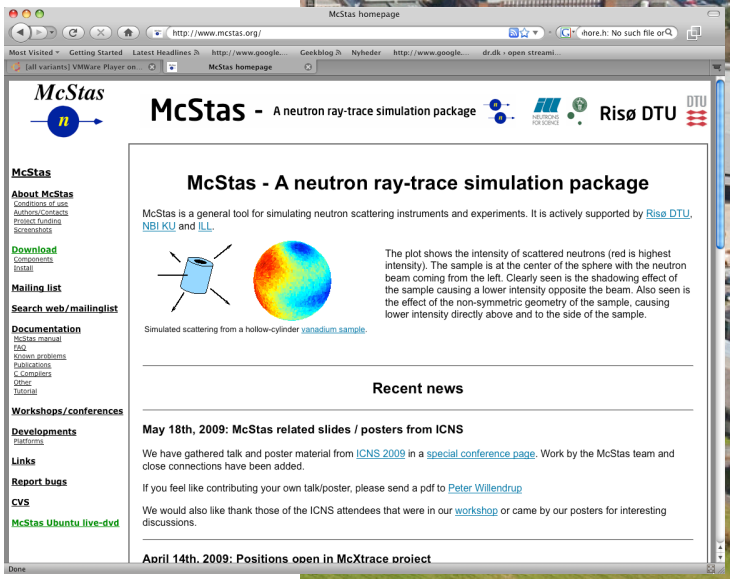
I x



McStas Introduction

- 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

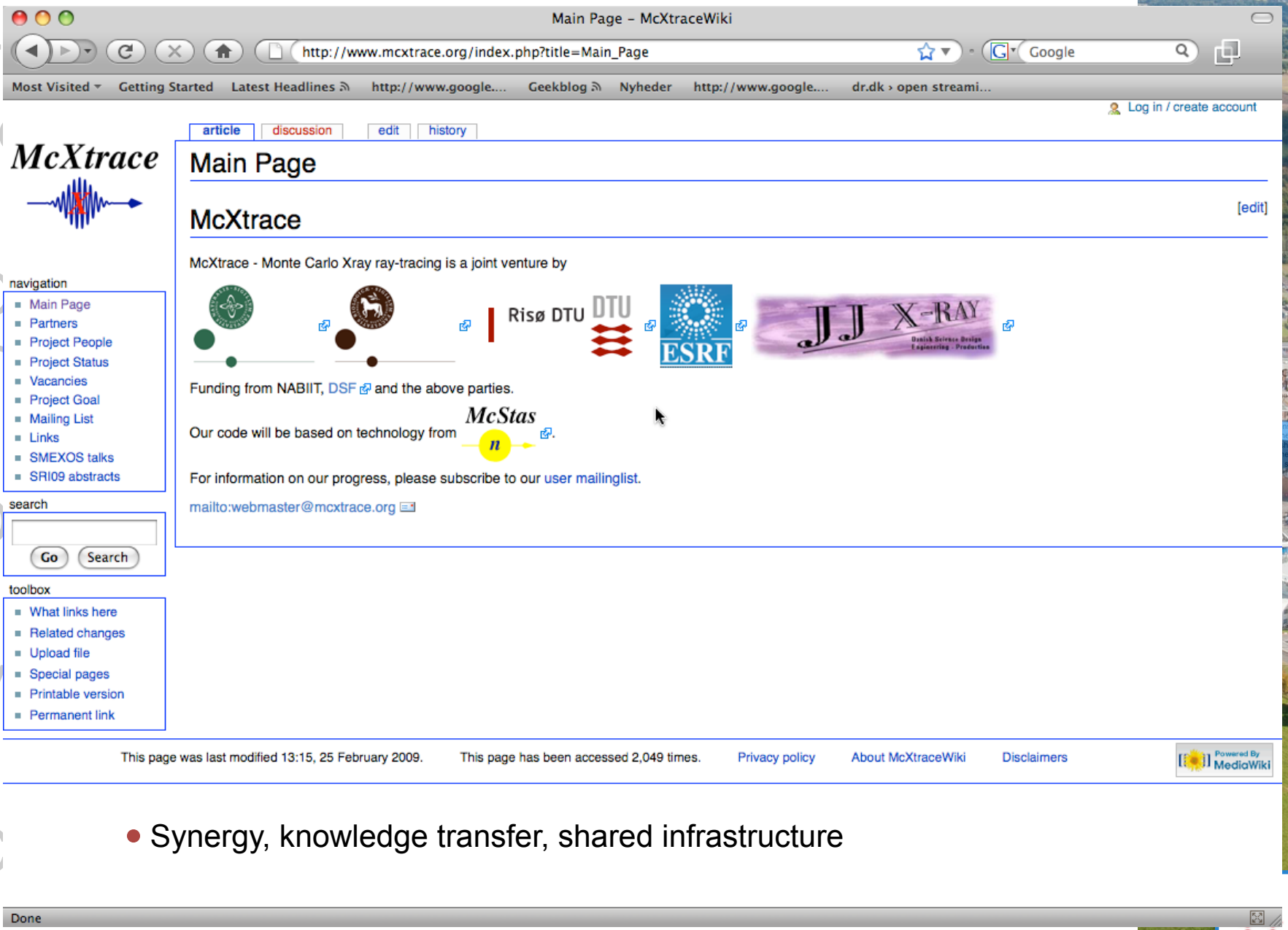
GNU GPL
license
Open Source



Project website at
http://www.mcstas.org

mcstas-users@mcstas.org mailinglist

McXtrace - since jan 2009 similar for X-rays

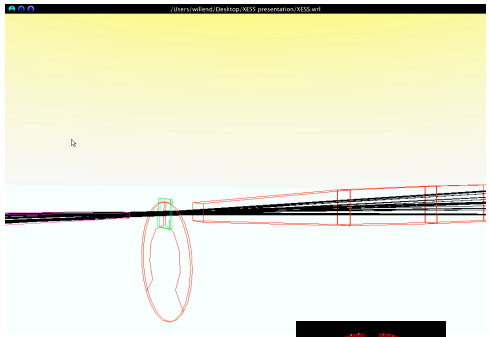


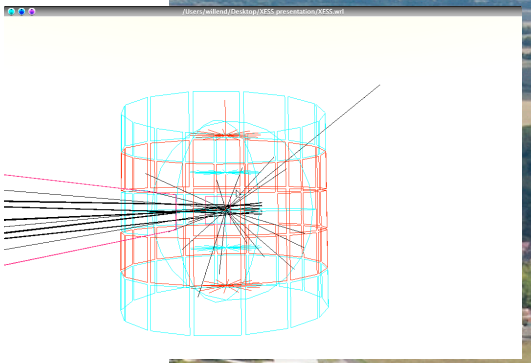
- Synergy, knowledge transfer, shared infrastructure

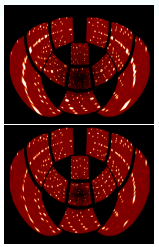
Used in many places

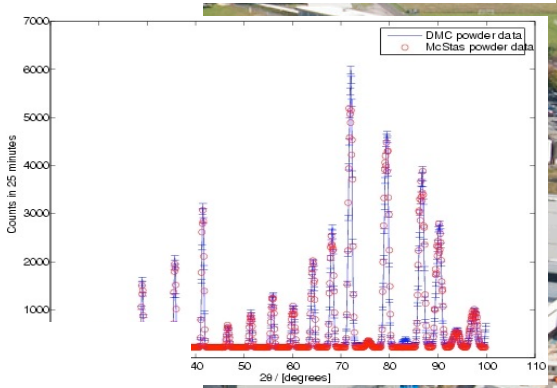
What is McStas used for?

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

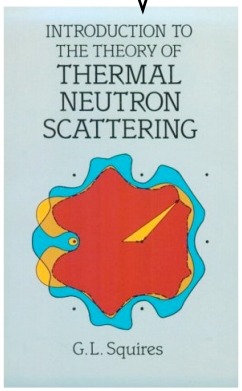


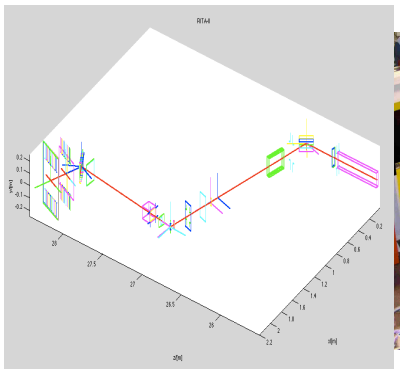


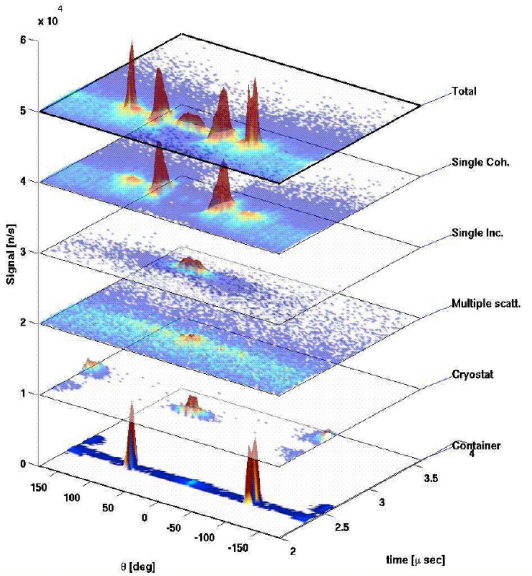




(KU, DTU)

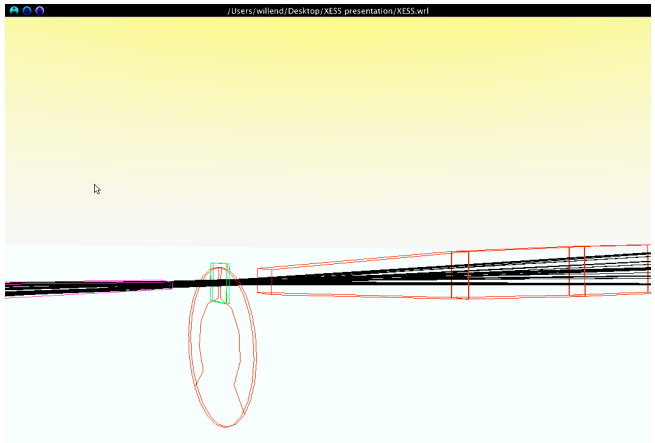


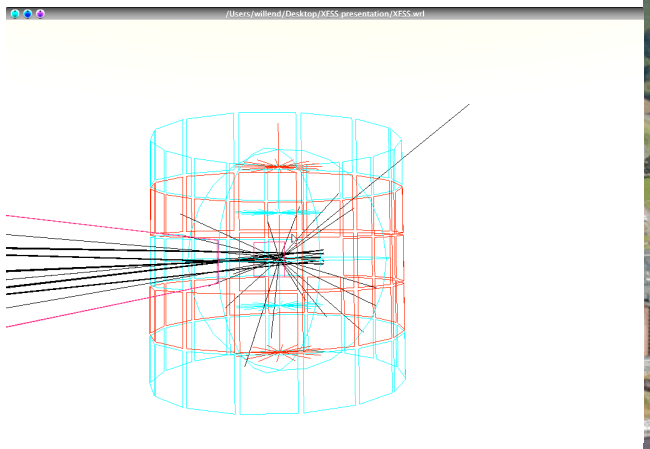


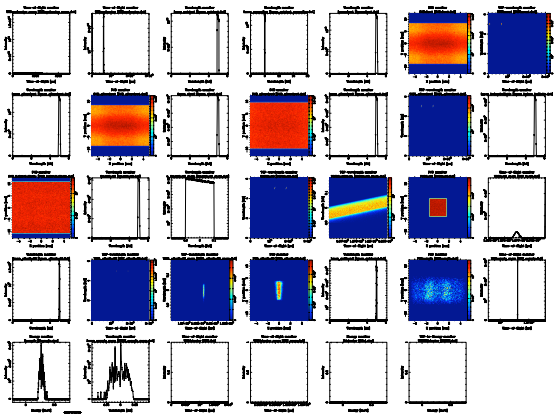


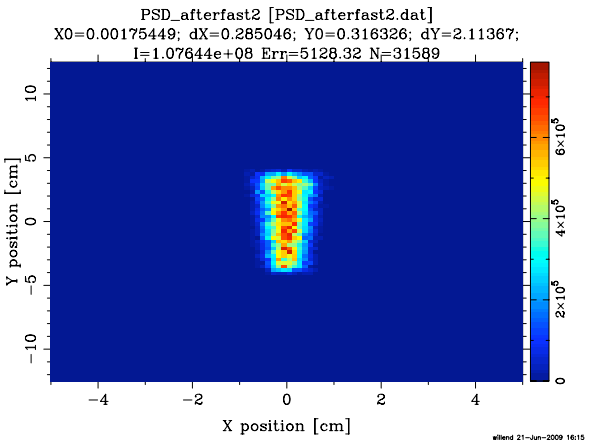
Instrumentation

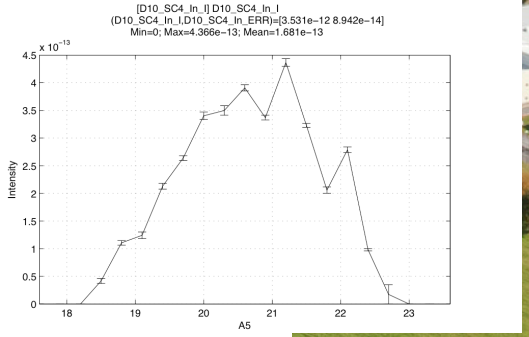
- Design and optimization of instruments







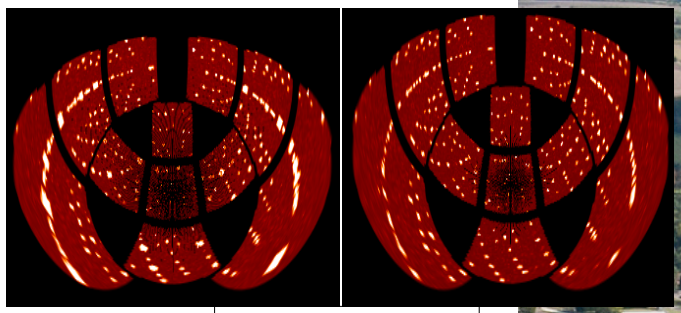




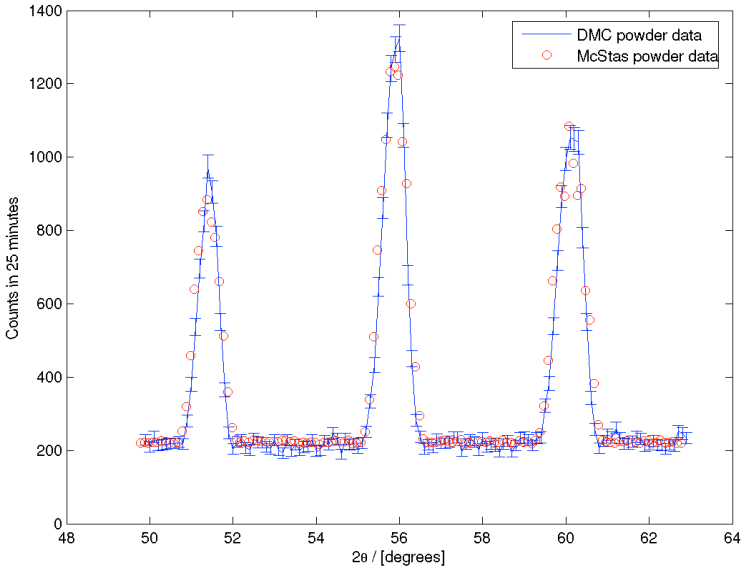
Virtual experiments (VE)

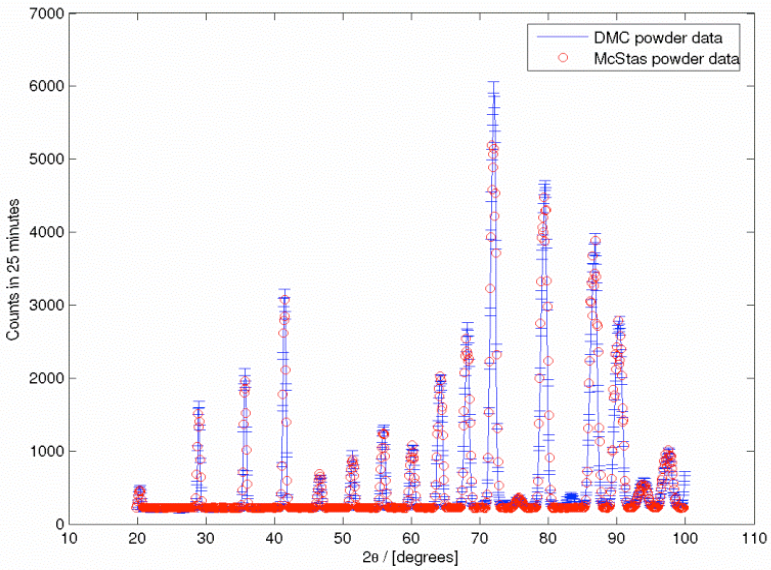
(definition:)

- Simulation of a complete experiment
- … from source to detector
- Ideally controlled like real experiment.
- Data analysed by ”real” analysis programs



A. Daud-Aladine, ISIS





P. Willendrup, Risø DTU; Uwe Filges, L. Keller, PSI

Data analysis (1)

(using VE techiques)

Virtual TOF exp. at IN6, ILL

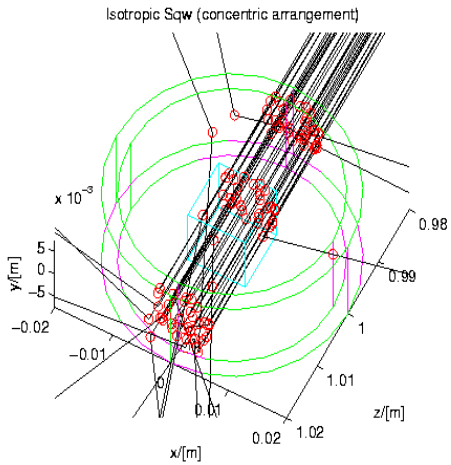
Liquid Ge sample

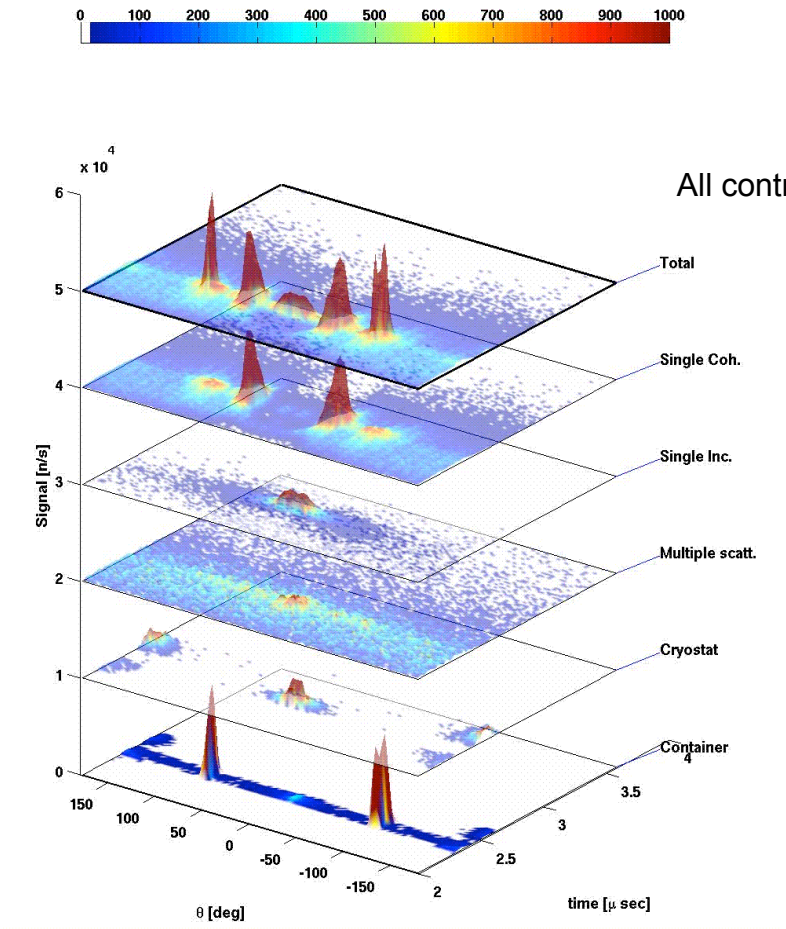
Coherent / incoherent

Multiple scattering

And sample environment

All contributions can be separated by VE !



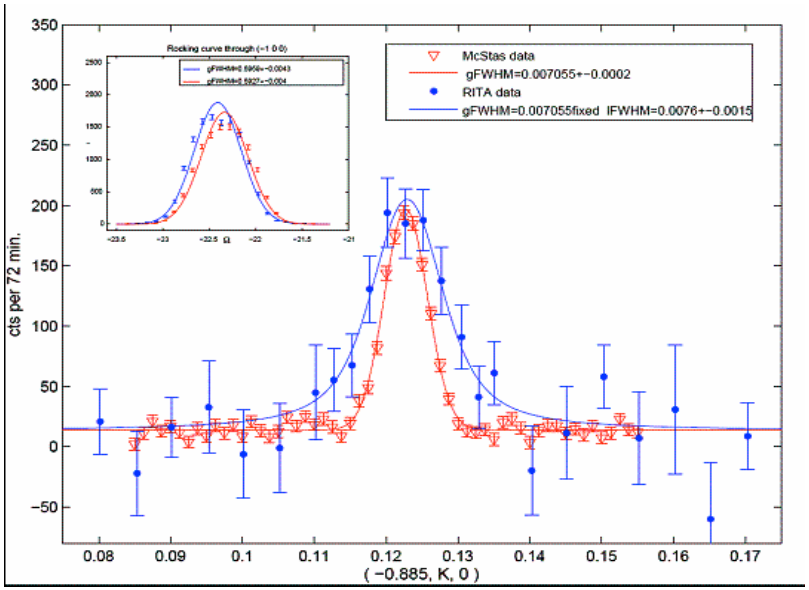


E. Farhi, ILL

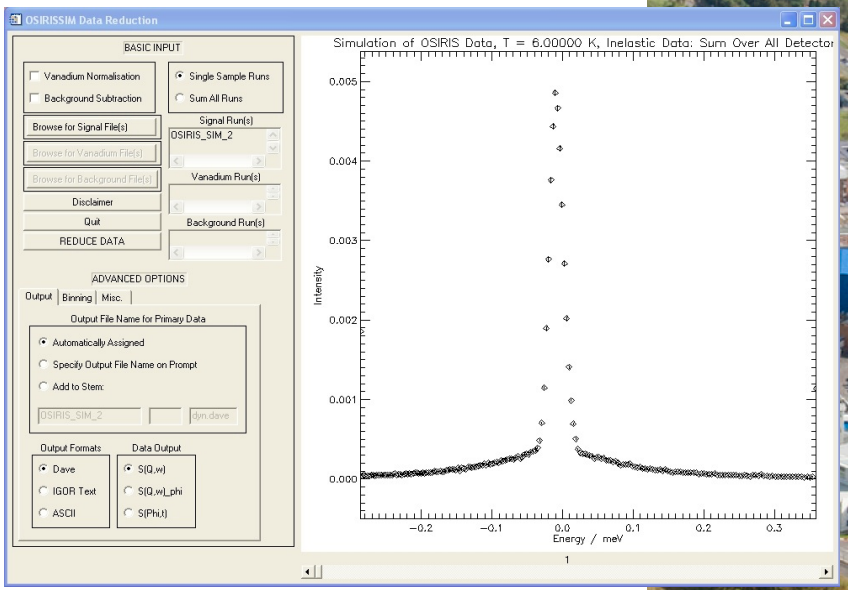
Data Analysis (2)

(using VE techniques)

- VE data has been used to test data analysis programs
- … and to check resolution effects



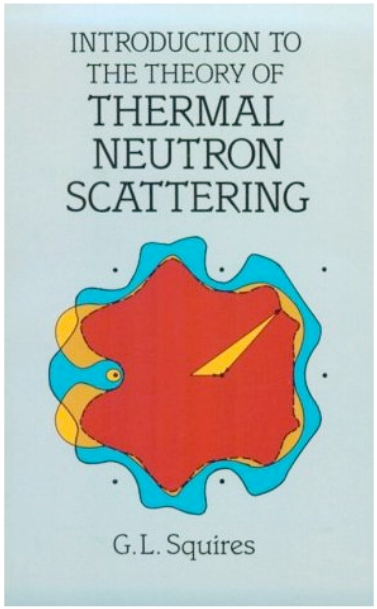
L. Udby, Risø-DTU

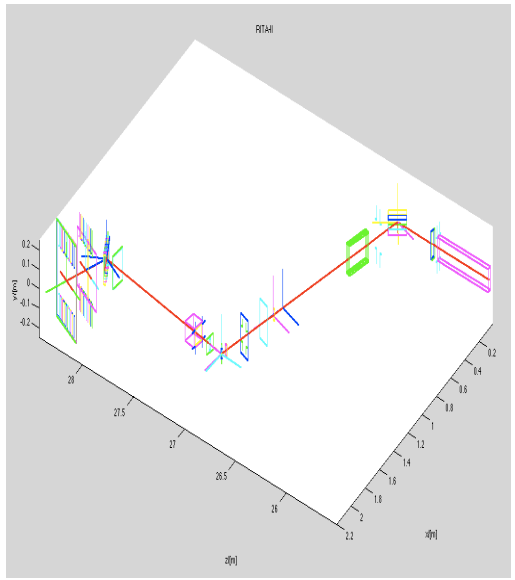


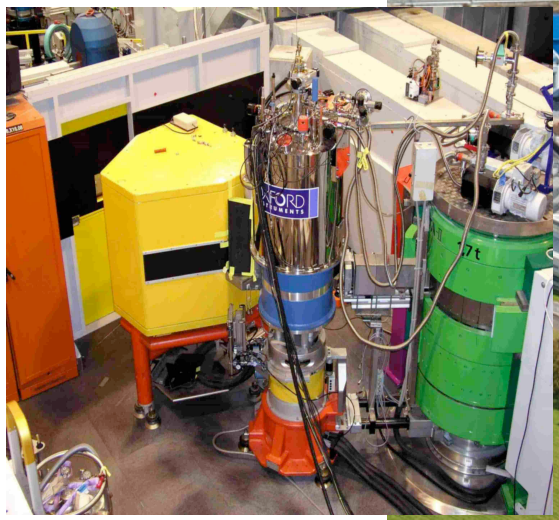
P. Tregenna-Piggott, PSI

Teaching / training purposes

- Workshops
- Teaching
  - University of Copenhagen course on Neutron Scattering 2005-, DTU 2011-

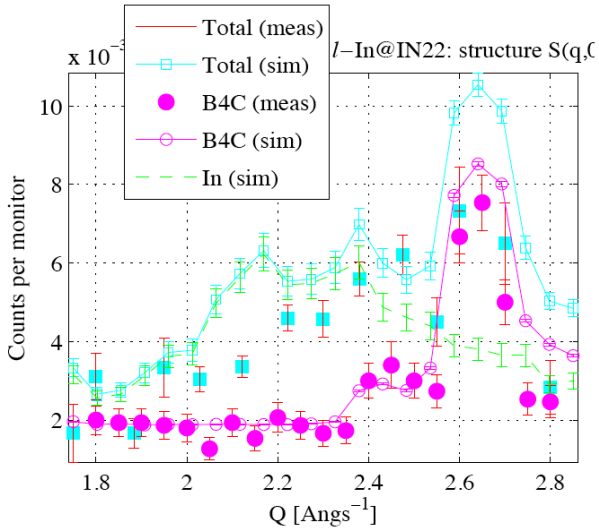




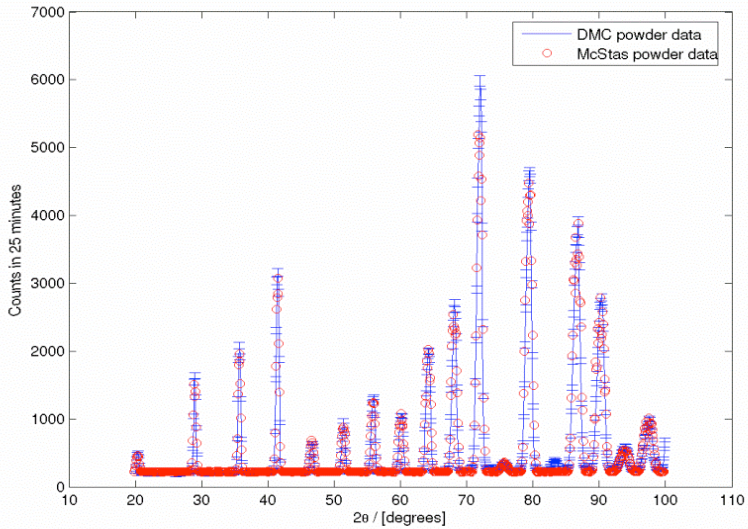


Reliability - cross comparisons

- 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

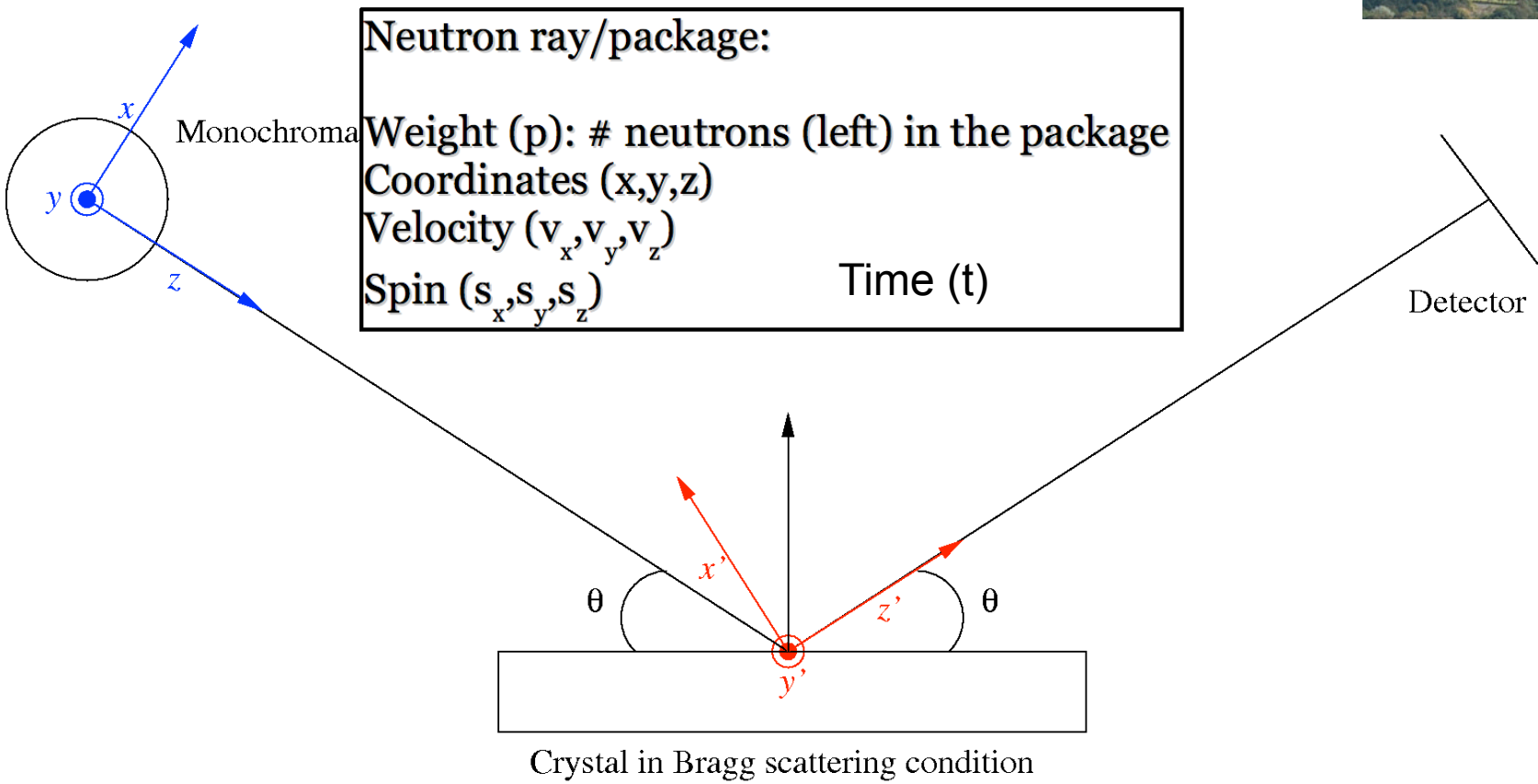


E. Farhi, P. Willendrup et al., in preparation

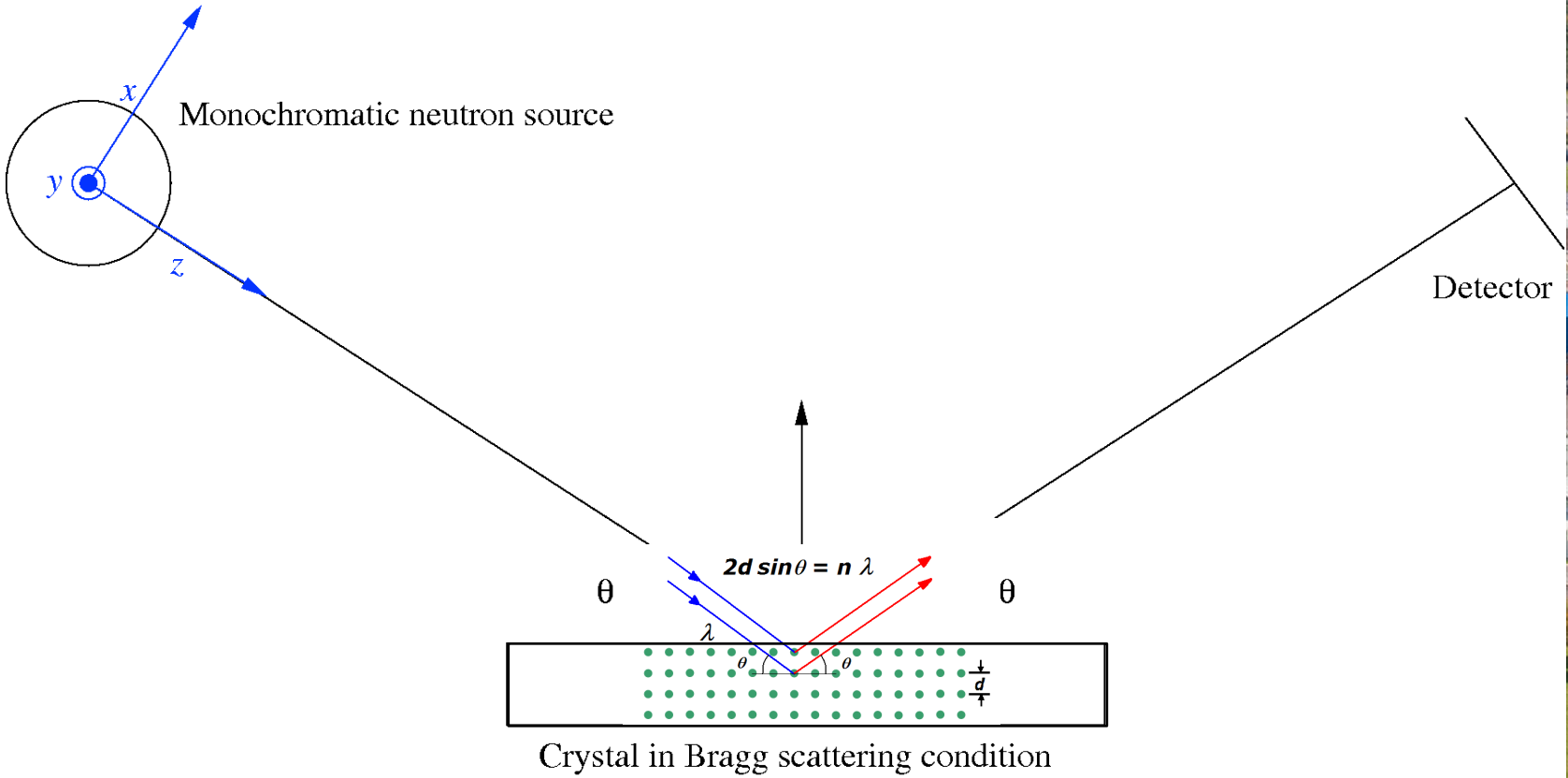


P. Willendrup et al., Physica B, 386, (2006), 1032.

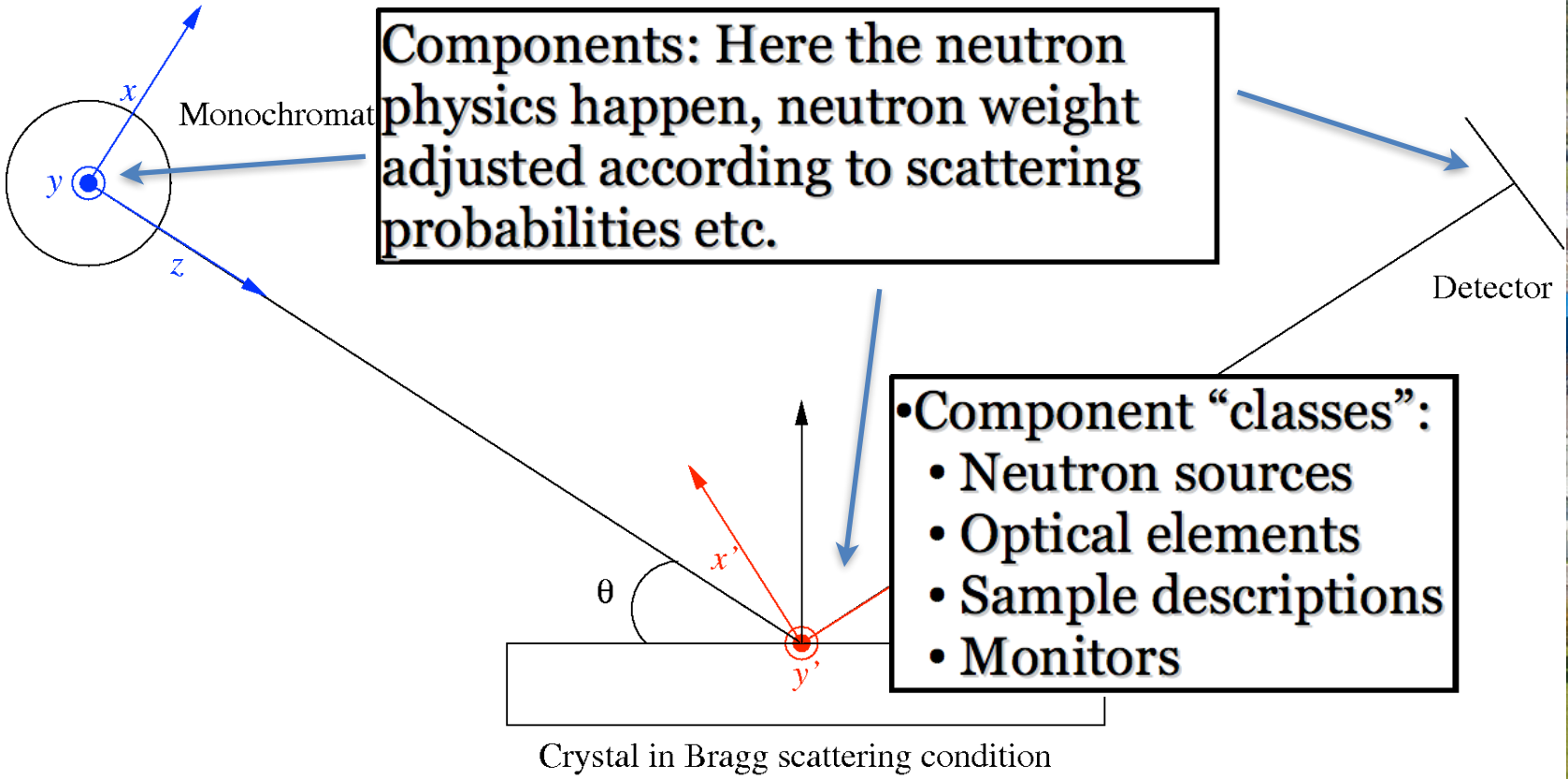
McStas: key concepts



McStas: key concepts

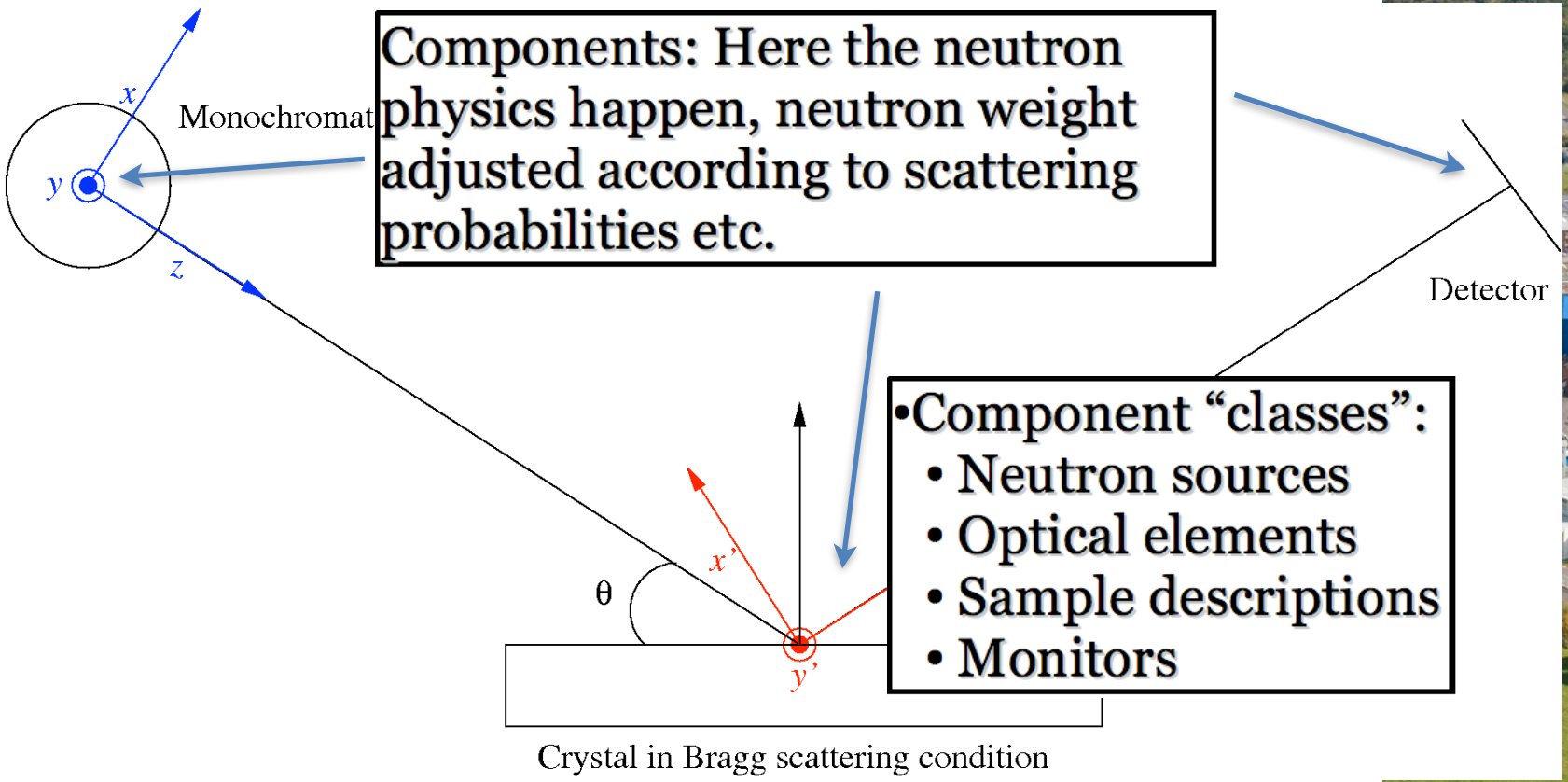


McStas: key concepts



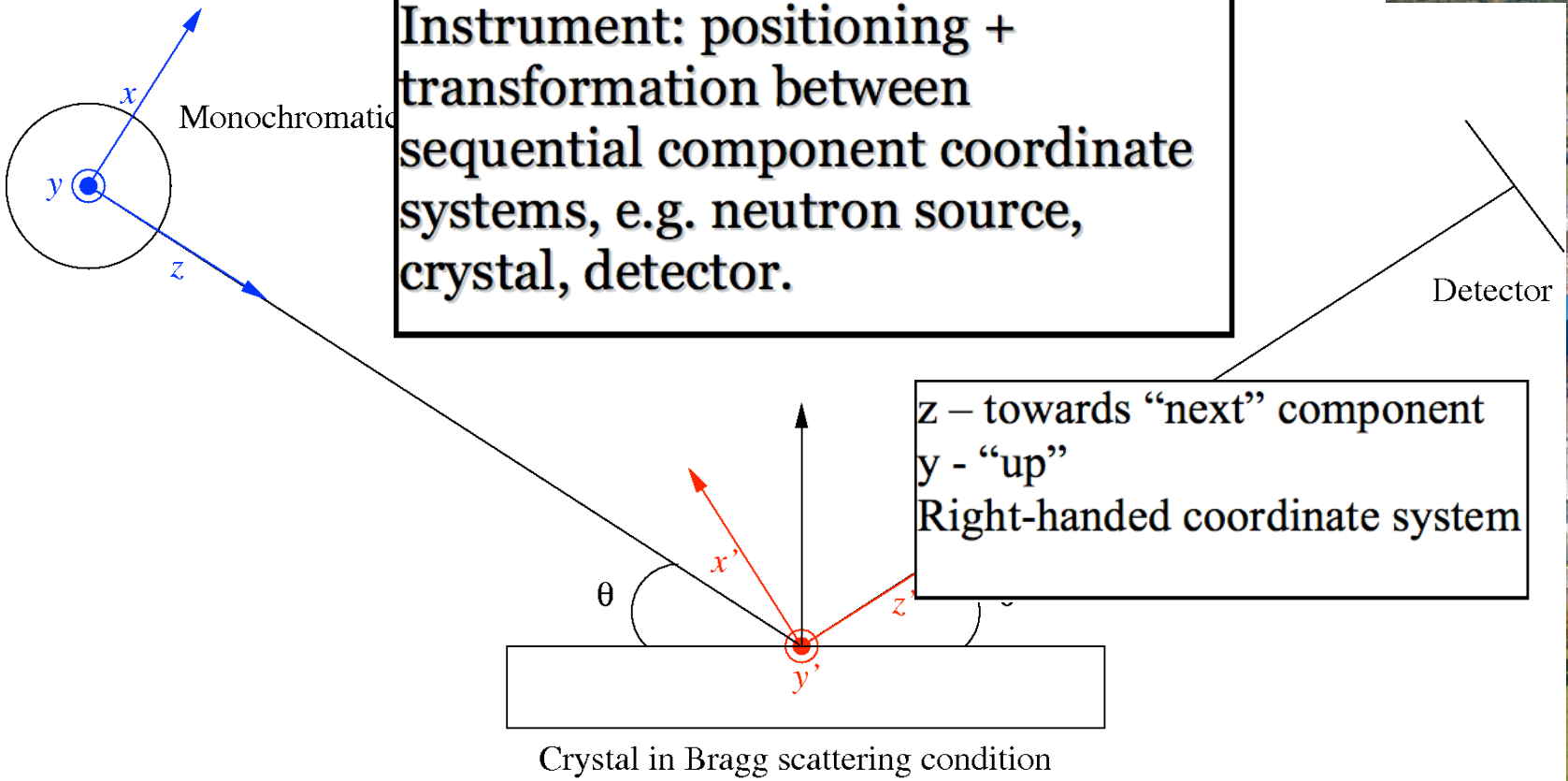
McStas: key concepts

Local, internal coordinate system!



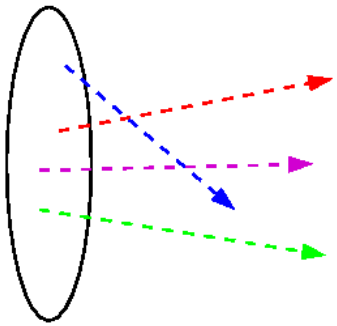
- Component "classes":
  - Neutron sources
  - Optical elements
  - Sample descriptions
  - Monitors

McStas: key concepts



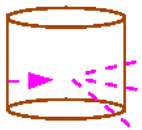
In the big picture…

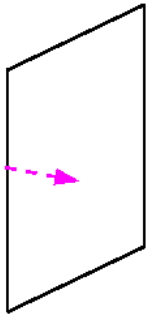
1. Particles emitted with random starting conditions via MC



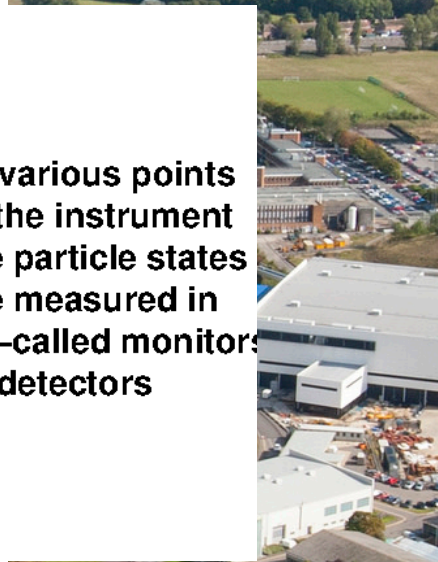
2. Particles are "ray–traced" through space

3. Will eventually meet other objects e.g. a studied experimental sample and get scattered via MC again





4. At various points in the instrument the particle states are measured in so–called monitors or detectors

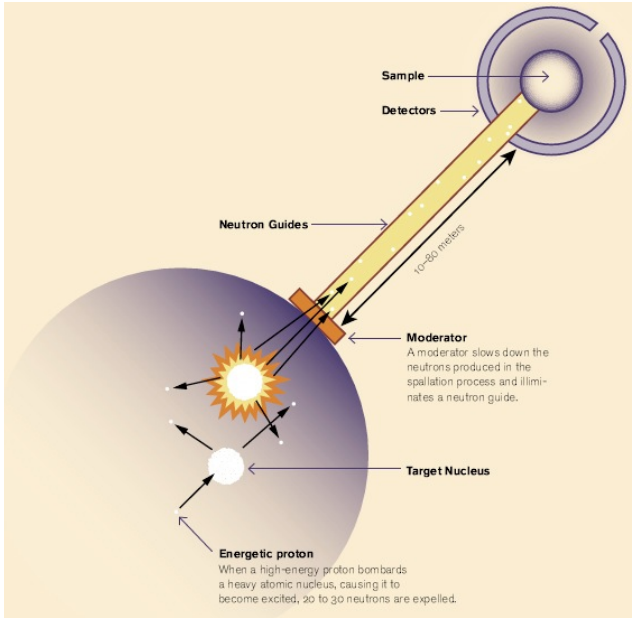


McStas overview

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

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

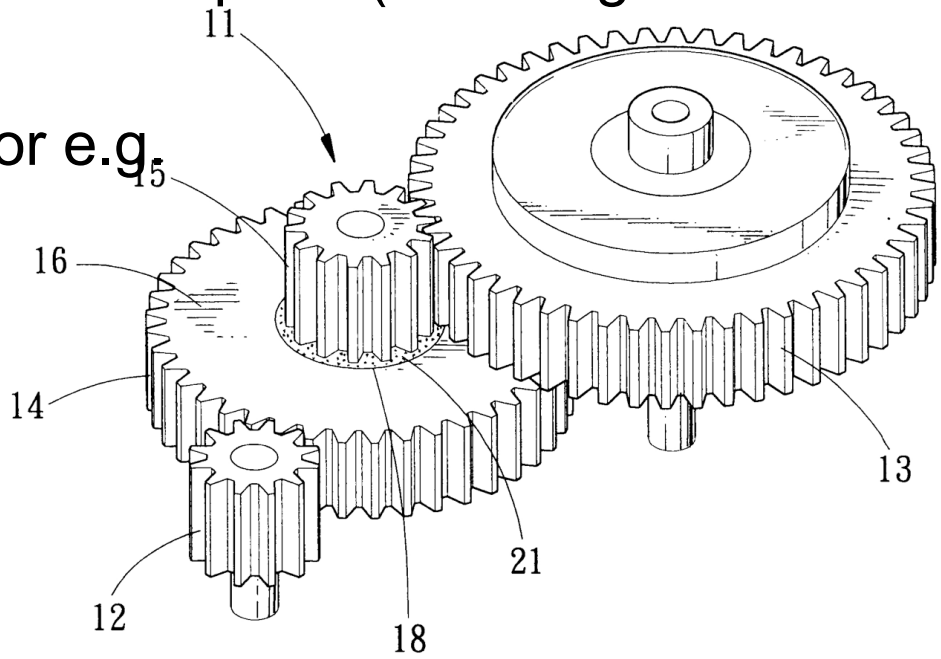
- 'Component' files (~100) inserted from library
  - Sources
  - Optics
  - Samples
  - Monitors
  - If needed, write your own comps



- 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)

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!

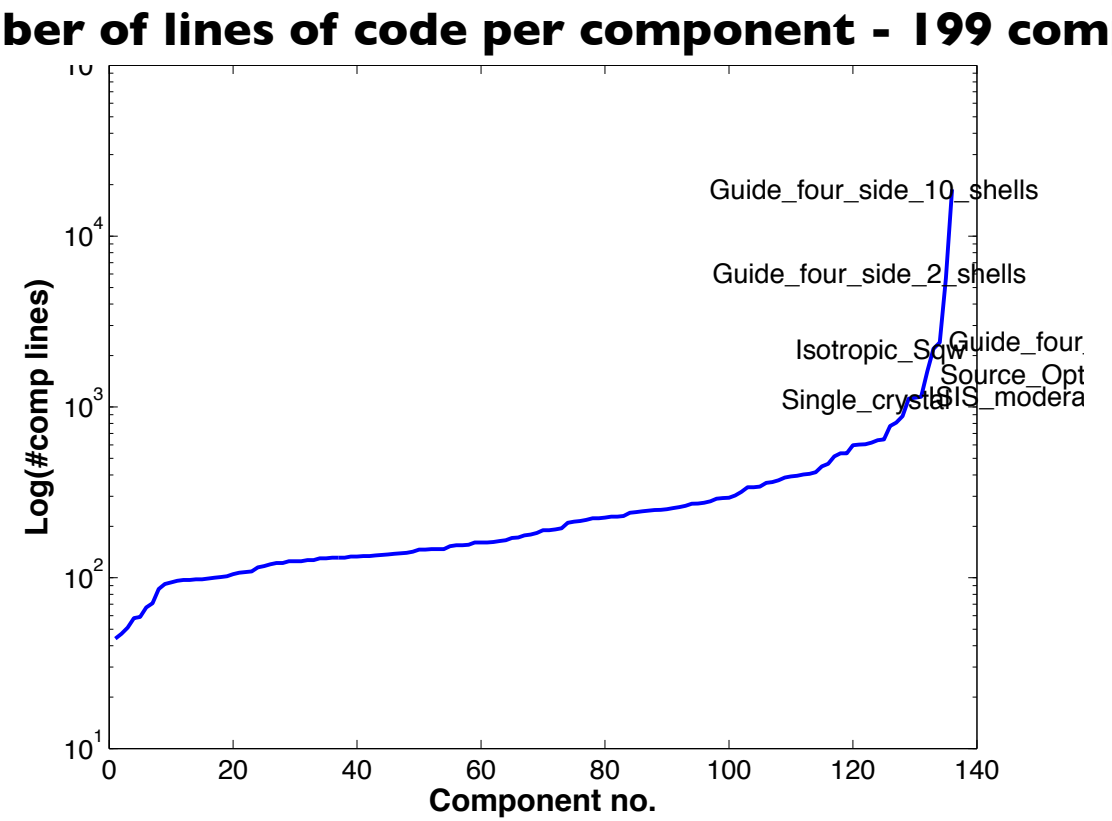
Input is .comp and .instr files + runtime functions for e.g. random numbers

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:

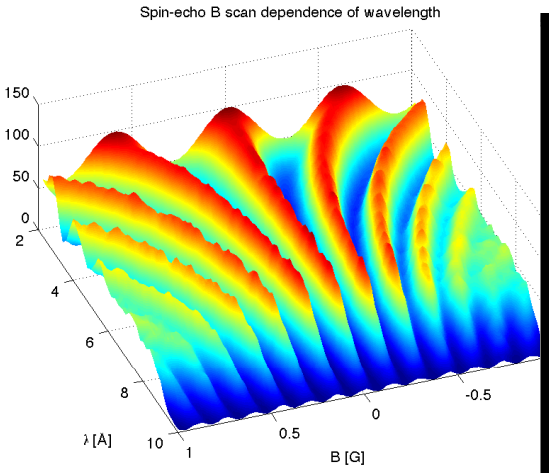


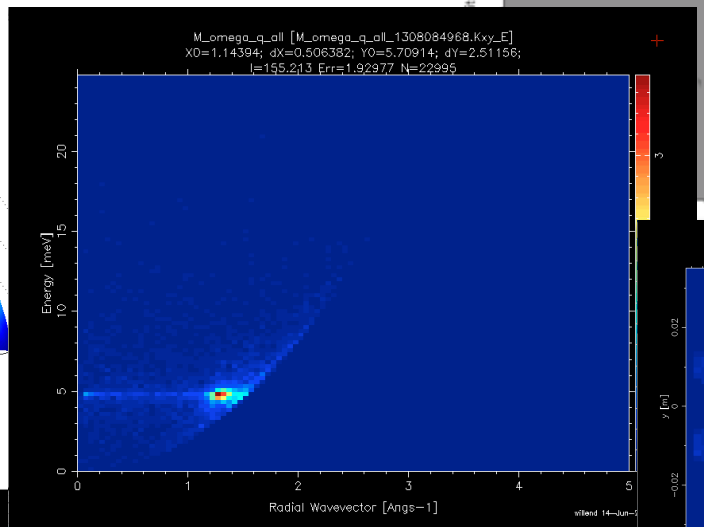
Including user contribs

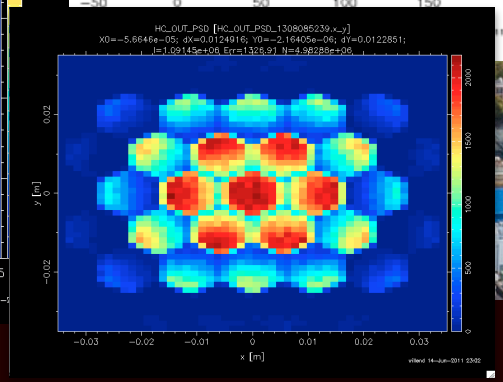
I Well-developed community support
- 30-40% of existing and new additions are from users
- No direct refereeing of the code, but these requirements:
  - At least one test-instrument
  - Meaningful documentation headers (in-code docs)
- Contributions go in dedicated contrib/ section of library

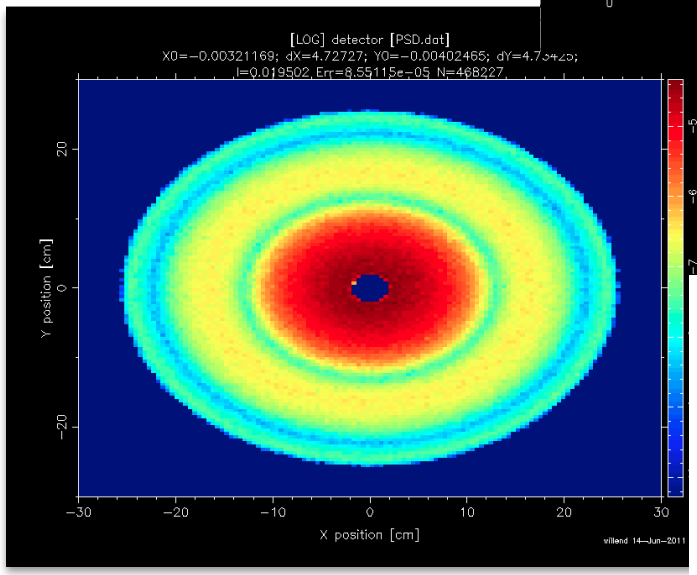
I Natural life-cycle of contrib's
- Bug-fixes are applied both by contributor and developers
- If contributor becomes unavailable either:
  - Many users of comp: Promote to official components, e.g. in optics/
  - Few/no users of comp: Move to obsolete/ until next major release

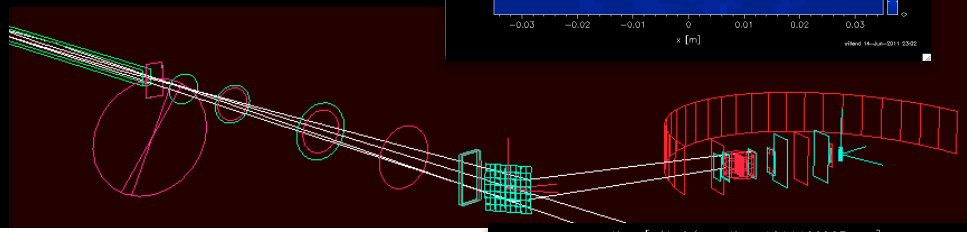
Example suite: ~140 instruments

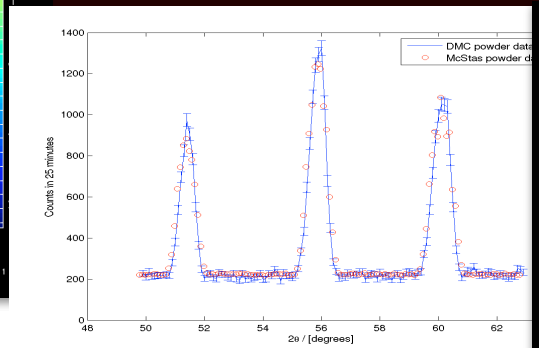


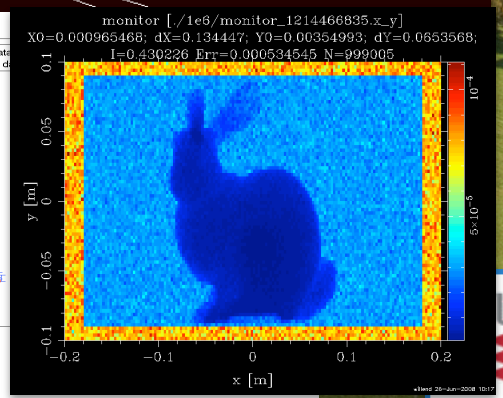












THIS IS NOT THE END

IT'S JUST THE BEGINNING