McStas

An introduction to

McStas – A neutron ray-trace simulation package

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RISØ

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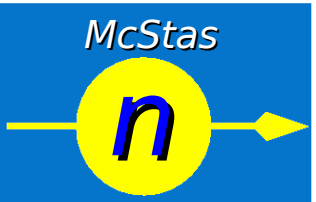
nmi3 EU Contract n°: HII3-CT-2003-505925

Agenda



- McStas
  - What is it?
  - What is it good for?
  - How is it done?
  - An online demo

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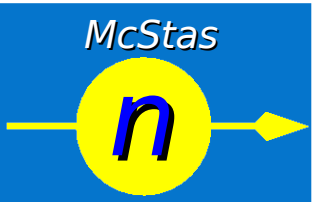
McStas introduction



- Flexible, general simulation utility for neutron scattering experiments.
- Original design for Monte carlo Simulation of triple axis spectrometers
- Developed at RISØ, ILL

GNU GPL license
Open Source
Please contribute!

- V. 1.0 by K Nielsen & K Lefmann (1998)
- Currently V. 1.9.1 (1.10 in beta – out 2006)
- Currently 2.5+1 people full time plus projects
- Apx. 100 users worldwide, some contributors
- Infrastructure:

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

neutron-mc@risoe.dk mailinglist
mcstas@risoe.dk developer contact

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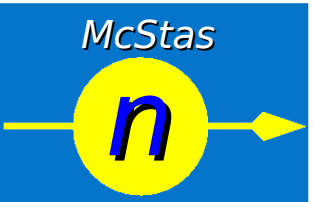
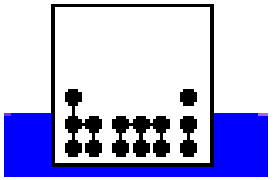
RISØ

McStas introduction



- Users at major labs







JAEA and KEK Joint Project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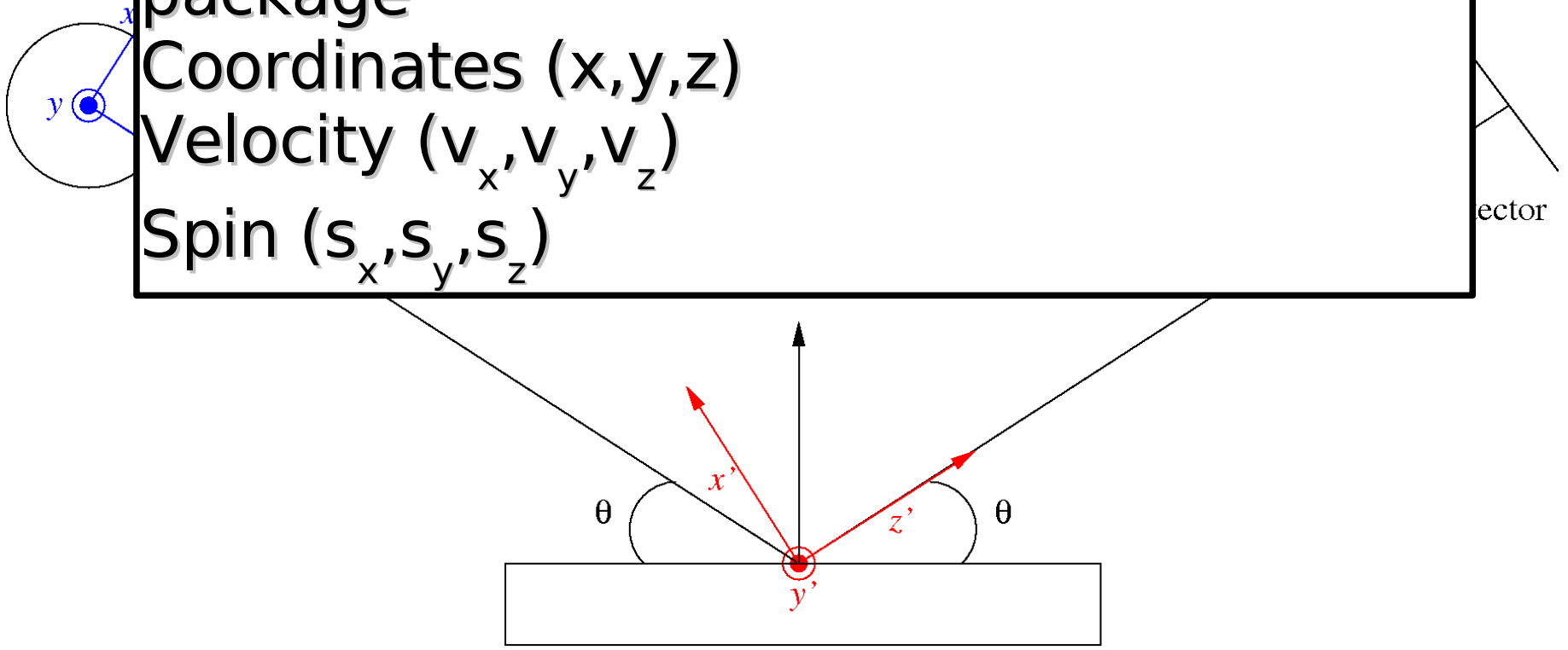
McStas introduction

Neutron ray/package:

Weight (p): # neutrons (left) in the package
Coordinates (x,y,z)
Velocity (v_x,v_y,v_z)
Spin (s_x,s_y,s_z)



Crystal in Bragg scattering condition

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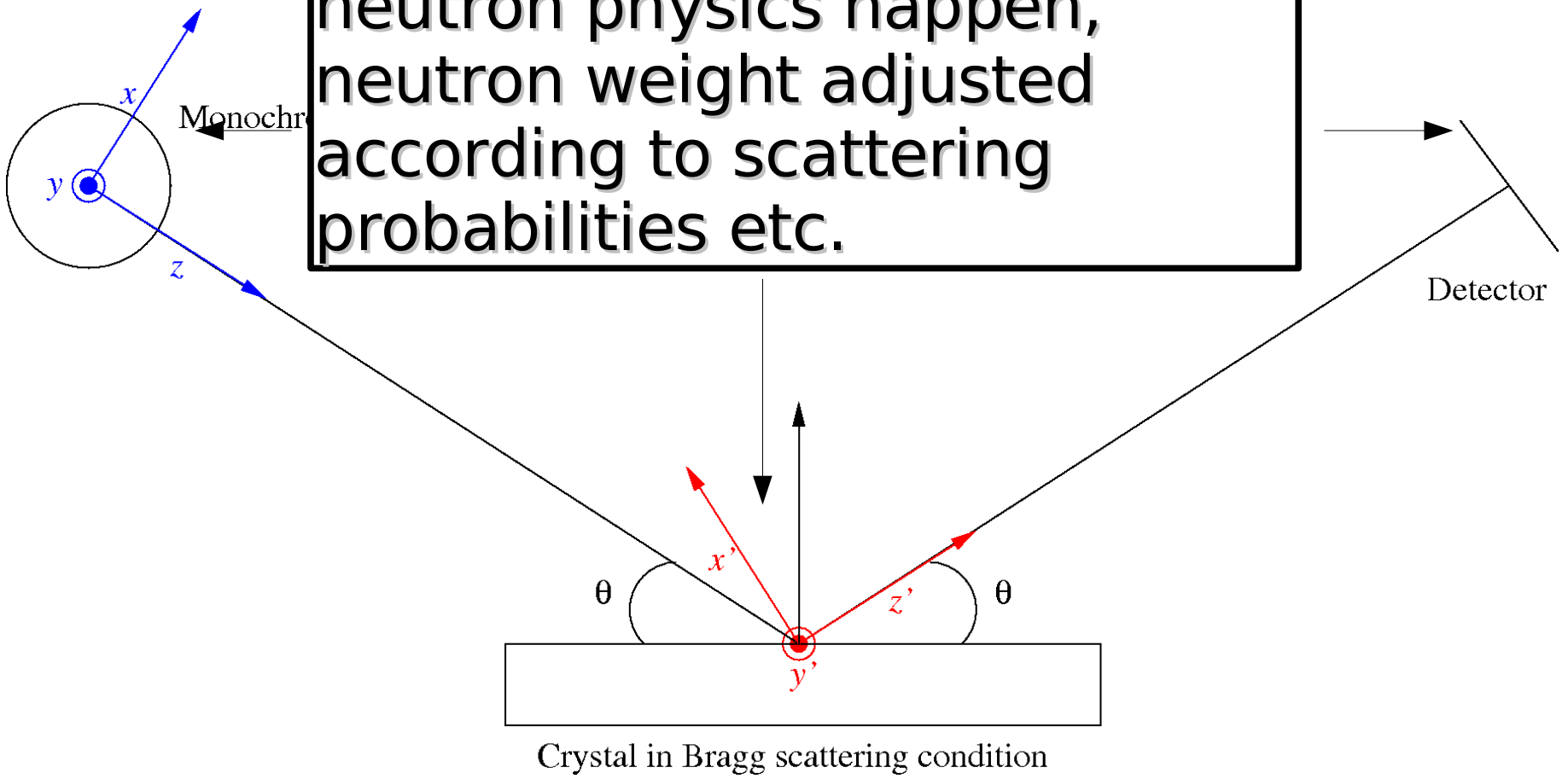
McStas introduction

Components: Here the neutron physics happen, neutron weight adjusted according to scattering probabilities etc.



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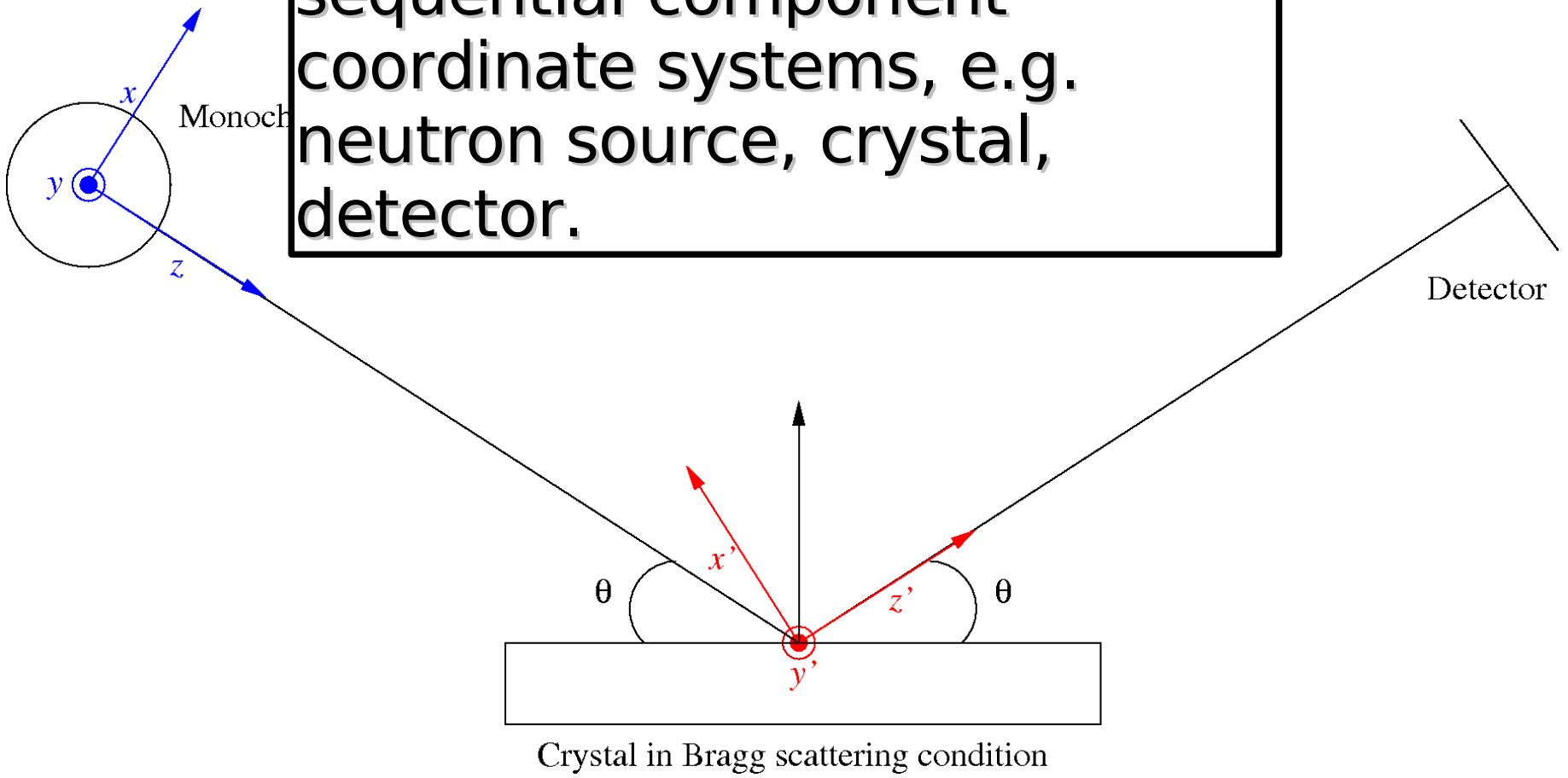
McStas introduction

Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.



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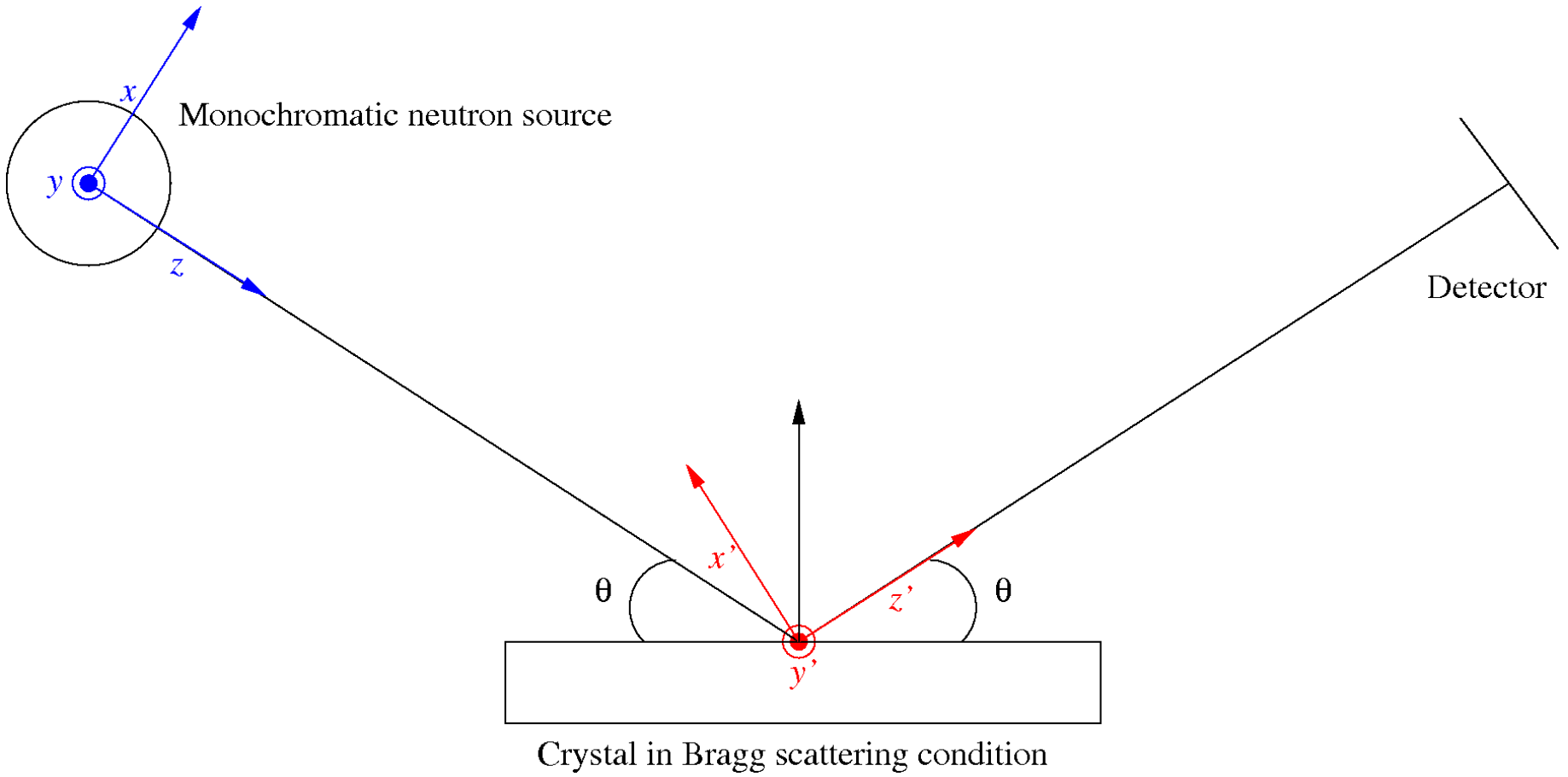
McStas introduction



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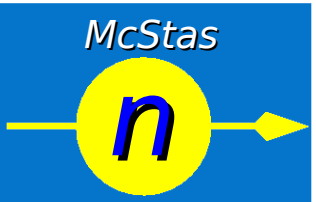
McStas introduction



- Portable code (Unix/Linux/Mac/Win32)
- Write in (simple) 'instrument' language
- 'Component' files (~100) inserted from library
  - Sources, optics, samples, monitors
- If needed, write your own components
- GUI / commandline functionality
- Tools for plotting and datahandling included

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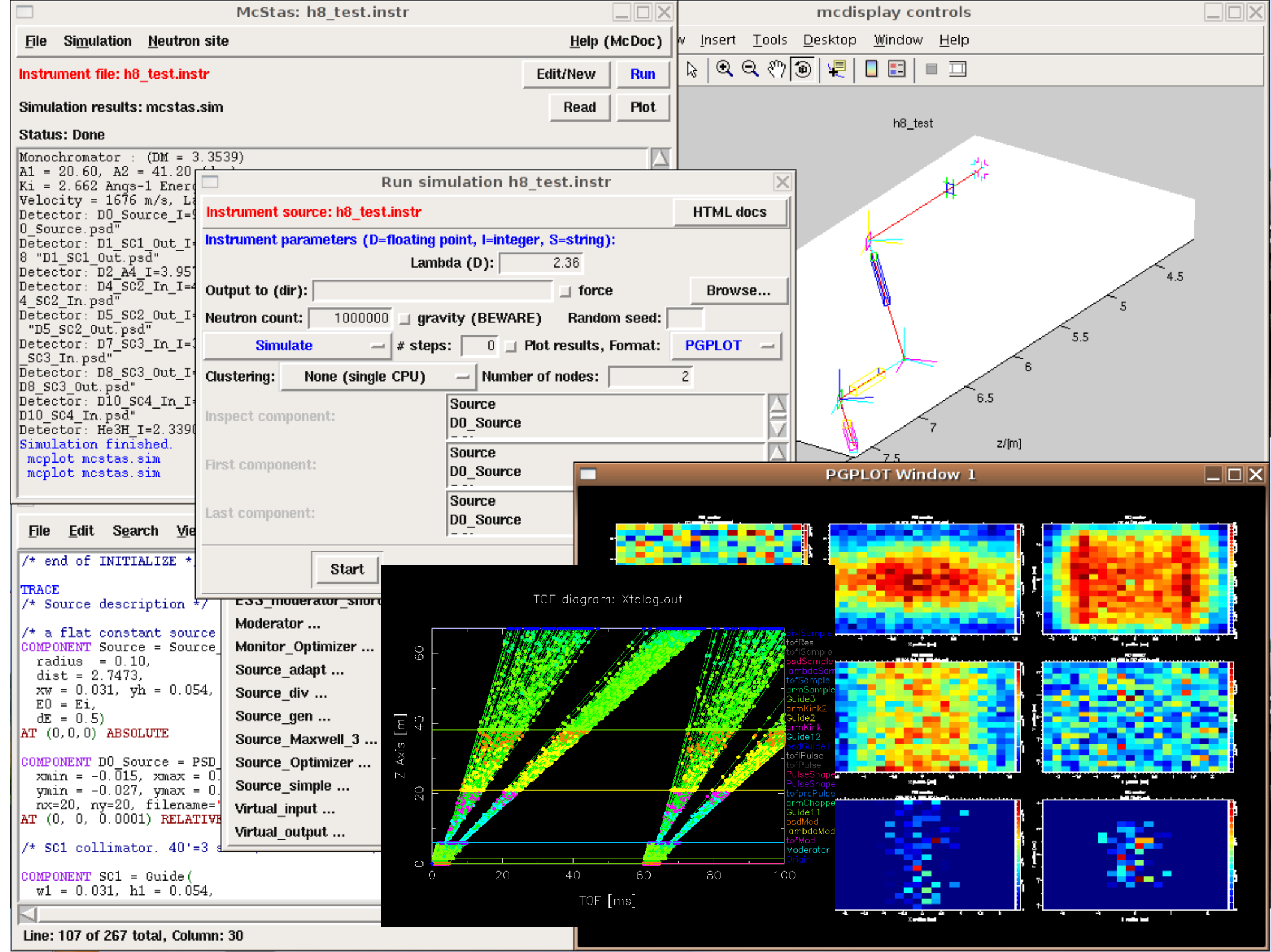
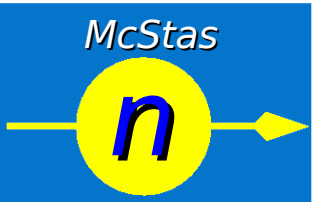

McStas: h8_test.instr
File Simulation Neutron site Help (McDoc)
Instrument file: h8_test.instr
Edit/New
Run
Simulation results: mcstas.sim
Read
Plot
Status: Done
Monochromator : (DM = 3.3539)
A1 = 20.60, A2 = 41.20
Ki = 2.662 Angs-1 Ener
Velocity = 1676 m/s, La
Detector: D0_Source_I=
0_Source.psd"
Detector: D1_SC1_Out_I=
8 "D1_SC1_Out.psd"
Detector: D2_A4_I=3.95
Detector: D4_SC2_In_I=
4_SC2_In.psd"
Detector: D5_SC2_Out_I=
"D5_SC2_Out.psd"
Detector: D7_SC3_In_I=
_SC3_In.psd"
Detector: D8_SC3_Out_I=
D8_SC3_Out.psd"
Detector: D10_SC4_In_I=
D10_SC4_In.psd"
Detector: He3H_I=2.339
Simulation finished.
mcplot mcstas.sim
mcplot mcstas.sim
Run simulation h8_test.instr
Instrument source: h8_test.instr
HTML docs
Instrument parameters (D=floating point, I=integer, S=string):
Lambda (D): 2.36
Output to (dir):
force
Browse...
Neutron count: 1000000
gravity (BEWARE)
Random seed:
Simulate
steps: 0
Plot results, Format: PGPLOT
Clustering: None (single CPU)
Number of nodes: 2
Inspect component:
First component:
Last component:
Source
D0_Source
Start
mcdisplay controls
Insert Tools Desktop Window Help
h8_test
z/[m]
4.5
5
5.5
6
6.5
7
7.5
File Edit Search
/* end of INITIALIZE *
TRACE
/* Source description */
/* a flat constant source
COMPONENT Source = Source_
radius = 0.10,
dist = 2.7473,
xw = 0.031, yh = 0.054,
E0 = Ei,
dE = 0.5)
AT (0,0,0) ABSOLUTE
COMPONENT D0_Source = PSD_
xmin = -0.015, xmax = 0.
ymin = -0.027, ymax = 0.
nx=20, ny=20, filename="
AT (0, 0, 0.0001) RELATIVE
/* SC1 collimator. 40'=3
COMPONENT SC1 = Guide(
w1 = 0.031, h1 = 0.054,
Moderator ...
Monitor_Optimizer ...
Source_adapt ...
Source_div ...
Source_gen ...
Source_Maxwell_3 ...
Source_Optimizer ...
Source_simple ...
Virtual_input ...
Virtual_output ...
Line: 107 of 267 total, Column: 30
TOF diagram: Xtalog.out
Z Axis [m]
TOF [ms]
0
20
40
60
80
100
PGPLOT Window 1

Implementation



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

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Implementation

McStas

```
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!

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McStas introduction

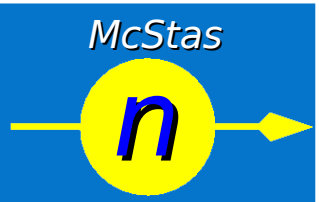
McStas

```
/*******************************************************************************
*
* 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!

McStas introduction




```
/* 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!

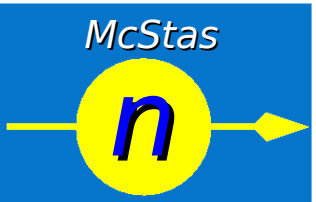
McStas is a (pre)compiler!

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.

What is McStas used for?



- Instrumentation
  - Planning
  - Optimization
- Data analysis
  - “I am seeing this strange effect, could it be due to....”
- Rehersal spectrometer for students and novice users

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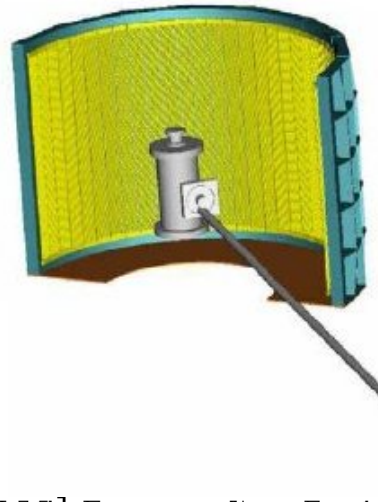
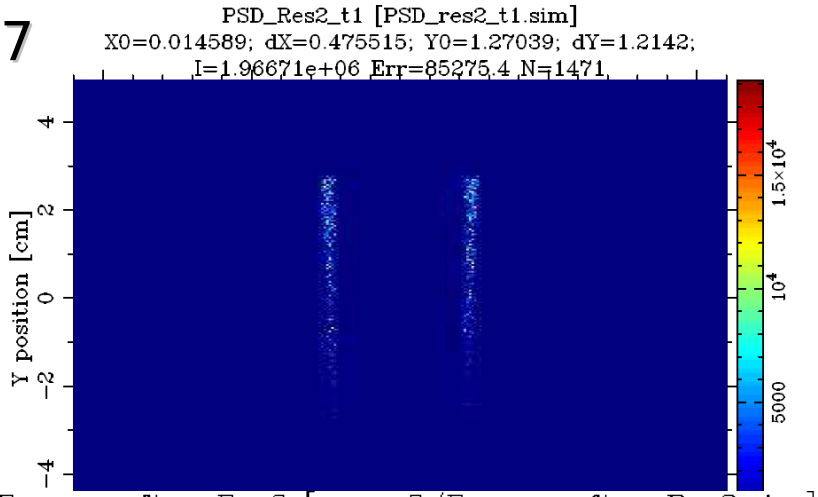
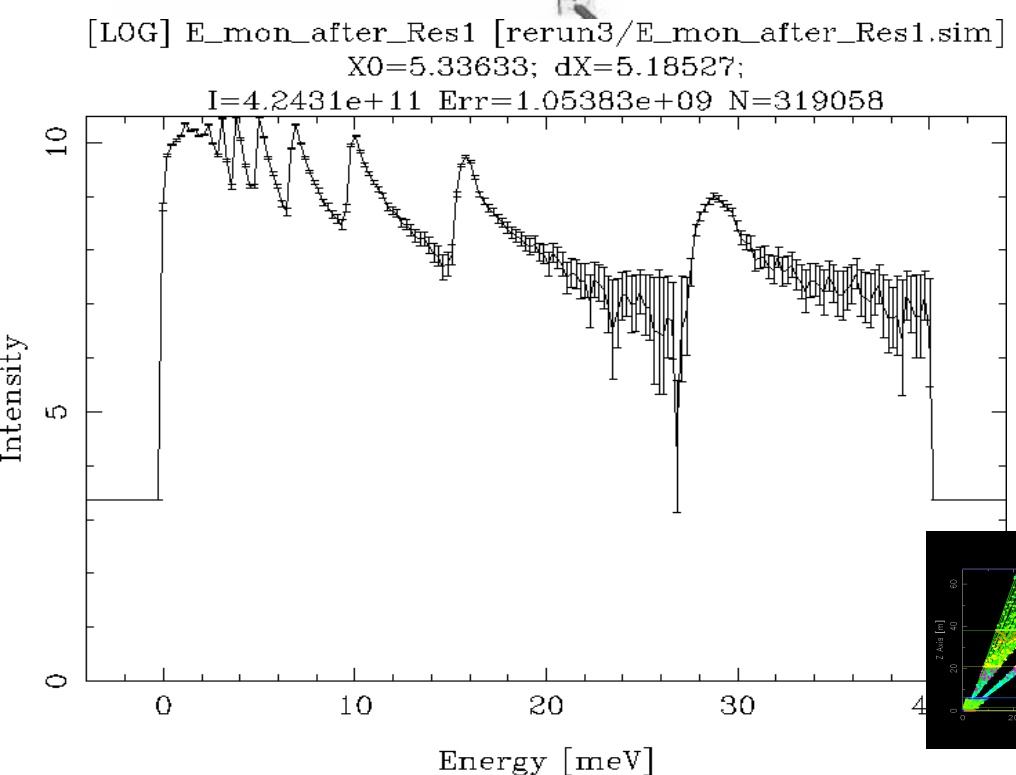
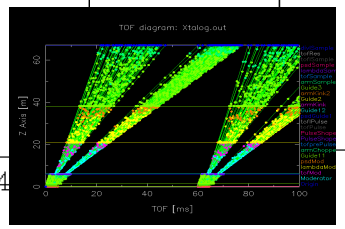
Time-Of-Flight (LET,ISIS)

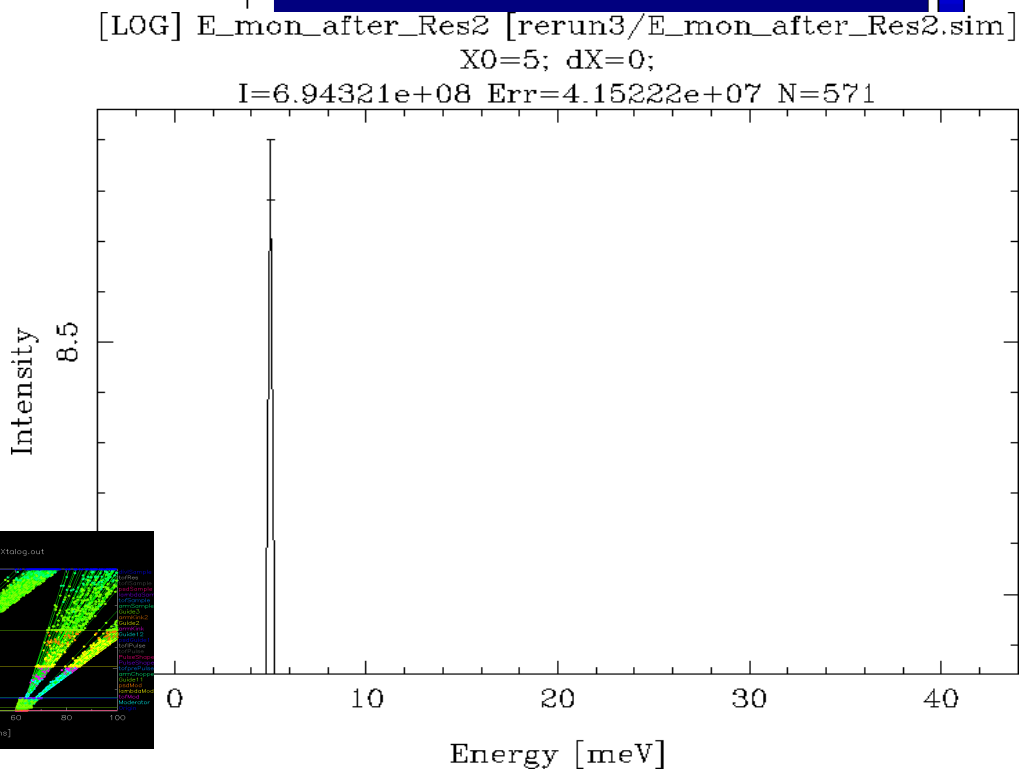


- Complicated design, total of 7 choppers!
- Notice effect of double resolution choppers below
- Subtle effects like of mismatch in chopper/guide geometry simulated (right)





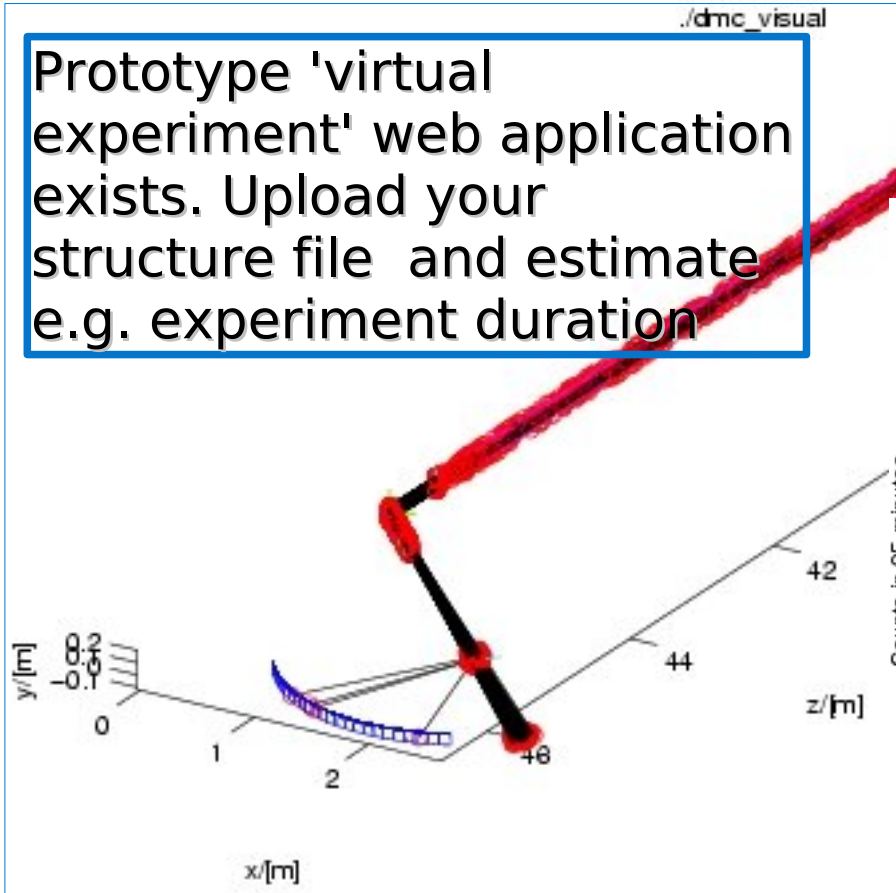




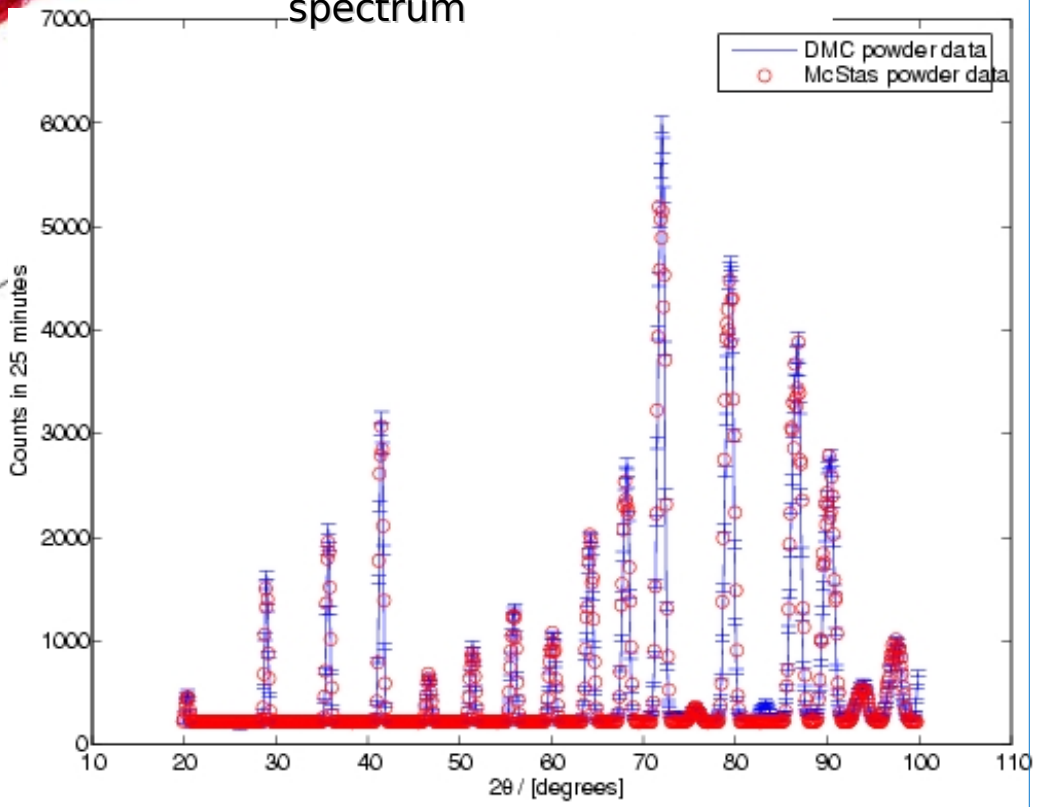
Powder Machine (DMC,PSI)

McStas

Prototype 'virtual experiment' web application exists. Upload your structure file and estimate e.g. experiment duration



$Na_2Ca_3Al_2F_{14}$ powder spectrum



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Peter Willendrup – McStas 1.10 MC wCNS, St. Charles, June 21st 2006
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Demo?

- Short online demo of McStas...

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