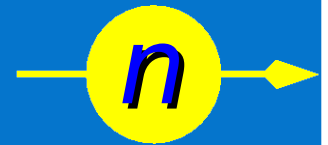# *McStas 1.10*

McStas 1.10

new release of the flexible neutron ray-tracing package - improved support for virtual experiments

*Peter Willendrup*, Peter Christiansen, Kim Lefmann
RISØ National Laboratory, Materials Research Department, DK-4000 Roskilde

Emmanuel Farhi, Klaus Lieutenant
Institut Laue-Langevin (ILL), 6 rue J. Horowitz, BP 156, 38042 Grenoble Cedex 9,France

- Short McStas introduction

  - Project structure, package overview

- Example simulations

  - TOF machines, Powder Diff

- New Features in 1.10

  - Language extensions, Polarisation support, Optimisation feature, reciprocal space calculator

- Conclusion
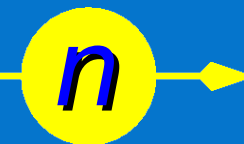
Short McStas introduction

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

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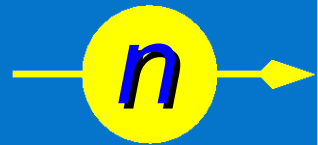- Apx. 100 users worldwide, some contributors
- Infrastructure:

GNU GPL license
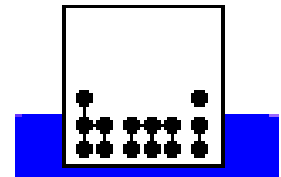Open Source
Please contribute!

Project website at   neutron-mc@risoe.dk mailinglist
http://www.mcstas.org   mcstas@risoe.dk developer contact

- Users at major labs

Monochromatic neutron source

Detector

Crystal in Bragg scattering condition
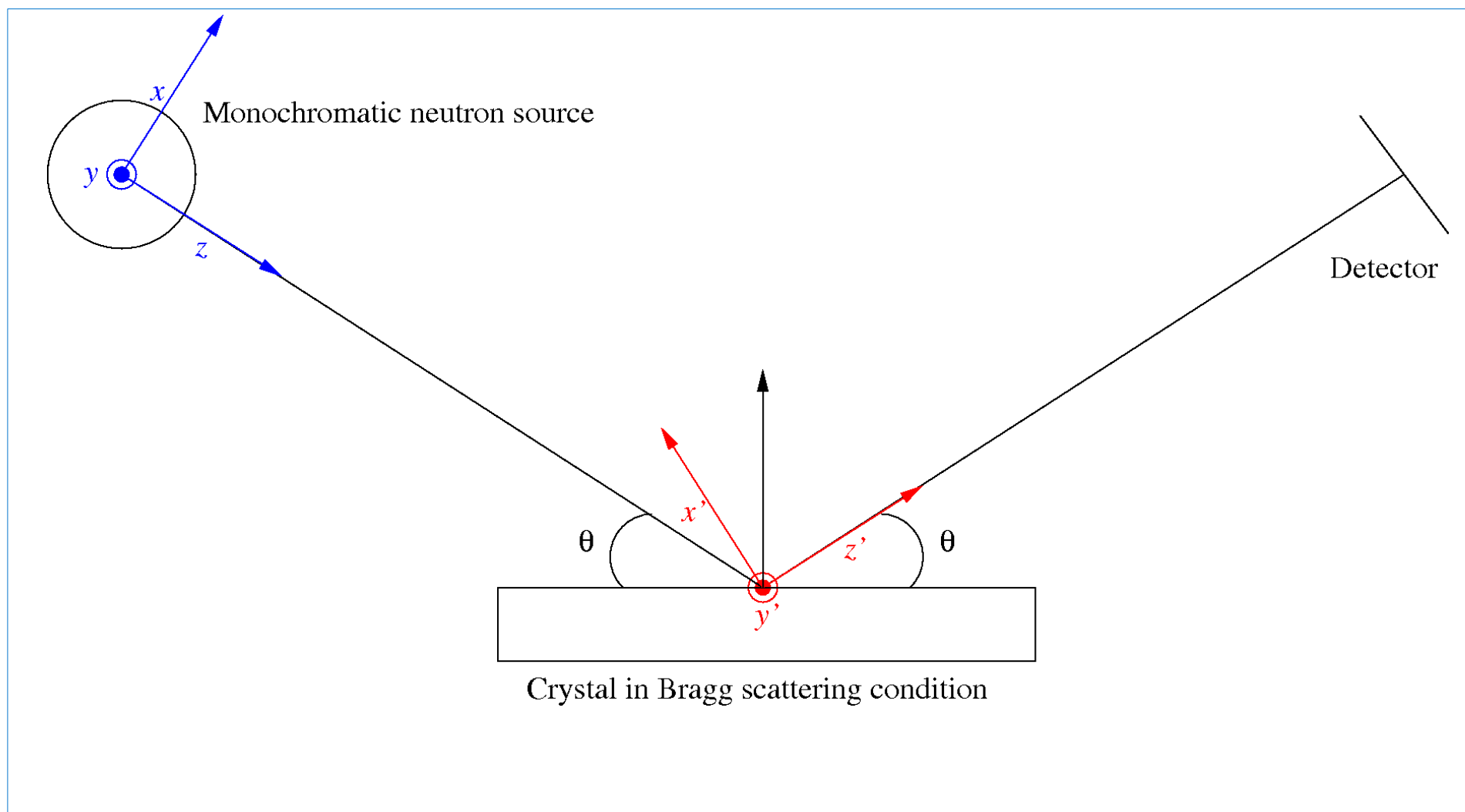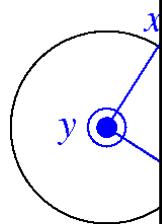
Short McStas introduction

Neutron ray/package:

Weight (p): # neutrons (left) in the package

Coordinates (x,y,z)

Velocity (v_x,v_y,v_z)
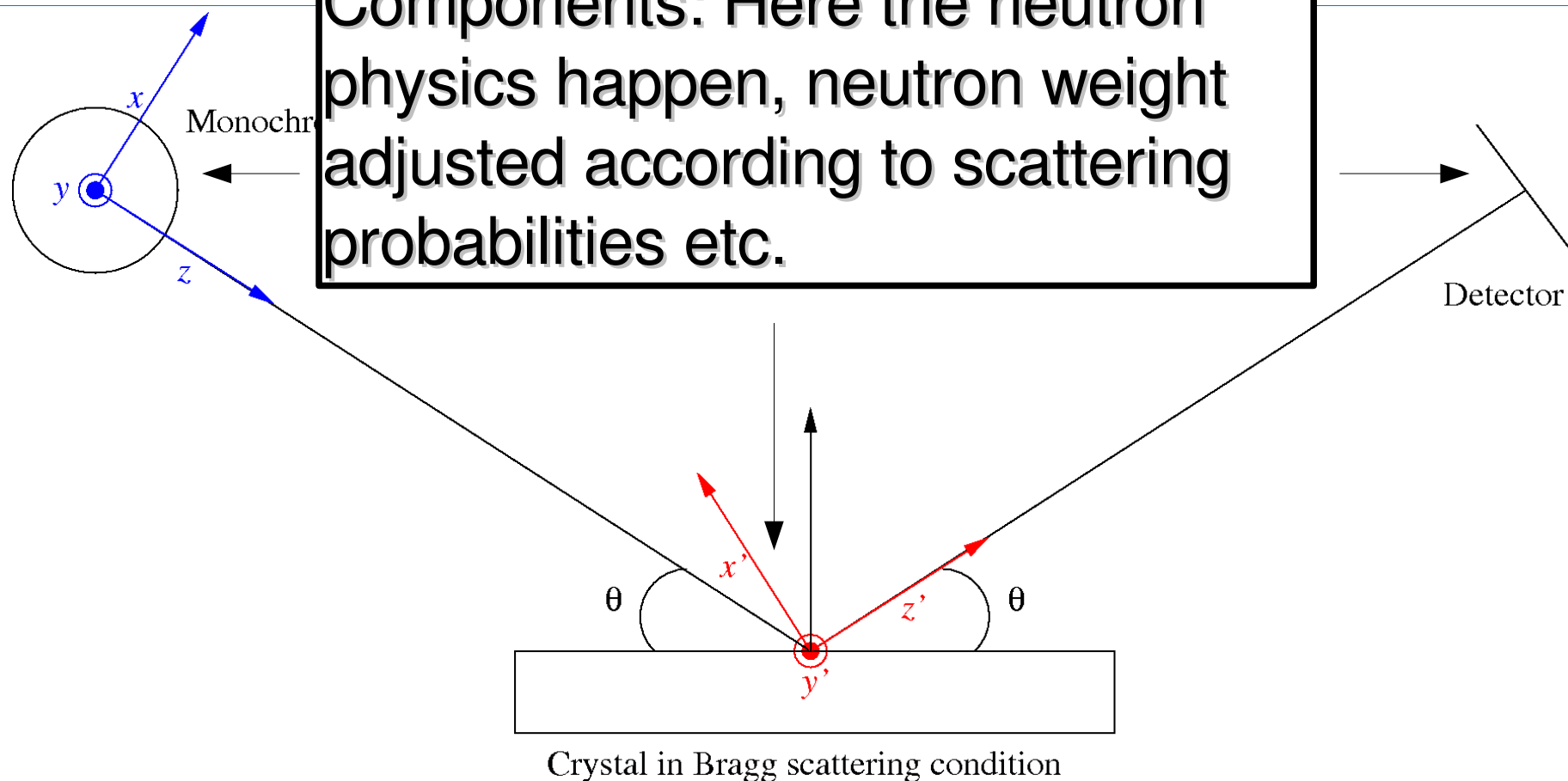
Spin (s_x,s_y,s_z)
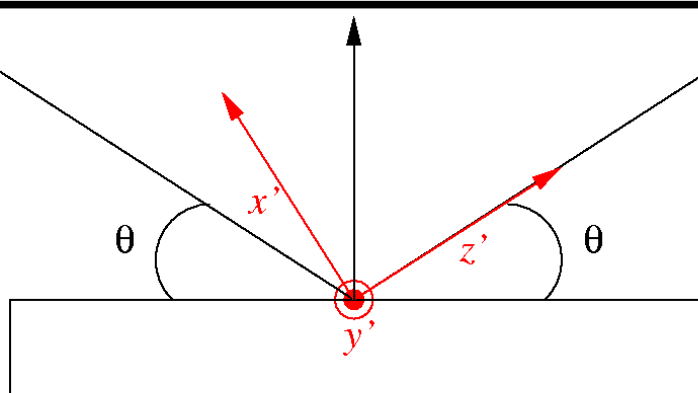
Crystal in Bragg scattering condition

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

Monochromator

x

y

z

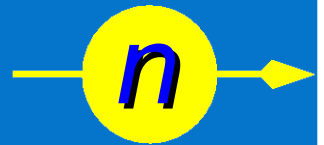x'

z'

y'

θ

θ

Detector

Crystal in Bragg scattering condition

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

x

Monoch...

y

z

θ

x'

z'

θ

y'

Detector

Crystal in Bragg scattering condition
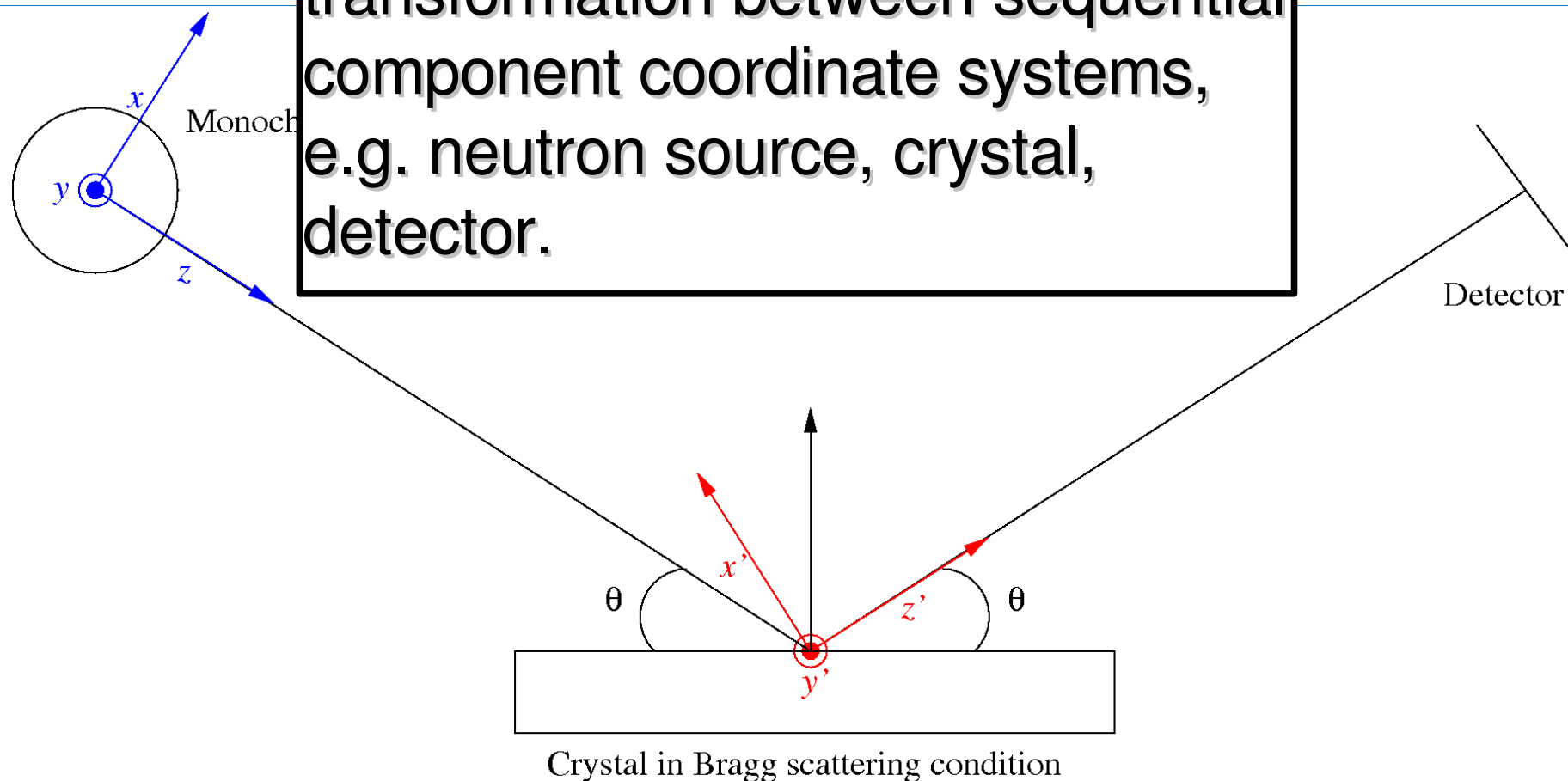
Short McStas introduction

- 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

File   Simulation   Neutron site   Help (McDoc)

Insert   Tools   Desktop   Window   Help

Instrument file: h8_test.instr

Edit/New   Run

Simulation results: mcstas.sim

Read   Plot

Status: Done

h8_test

```
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=9
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
4_SC2_In.psd"
Detector: D5_SC2_Out_I=
 "D5_SC2_Out.psd"
Detector: D7_SC3_In_I=3
_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: Source / D0_Source / - --

First component: Source / D0_Source / - --

Last component: Source / D0_Source / - --

Start

4.5

5

5.5

6

6.5

7

7.5

z/[m]

PGPLOT Window 1

File   Edit   Search   Vie

```
/* 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 s

COMPONENT SC1 = Guide(
  w1 = 0.031, h1 = 0.054,
```

ESS_moderator_short ...
Moderator ...
Monitor_Optimizer ...
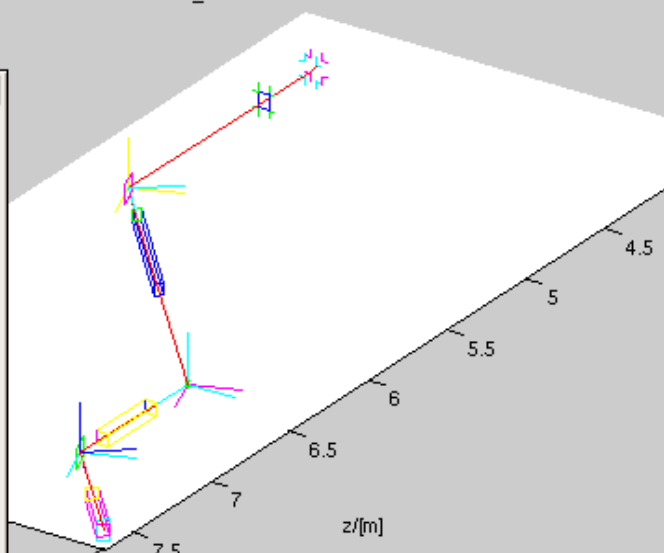Source_adapt ...
Source_div ...
Source_gen ...
Source_Maxwell_3 ...
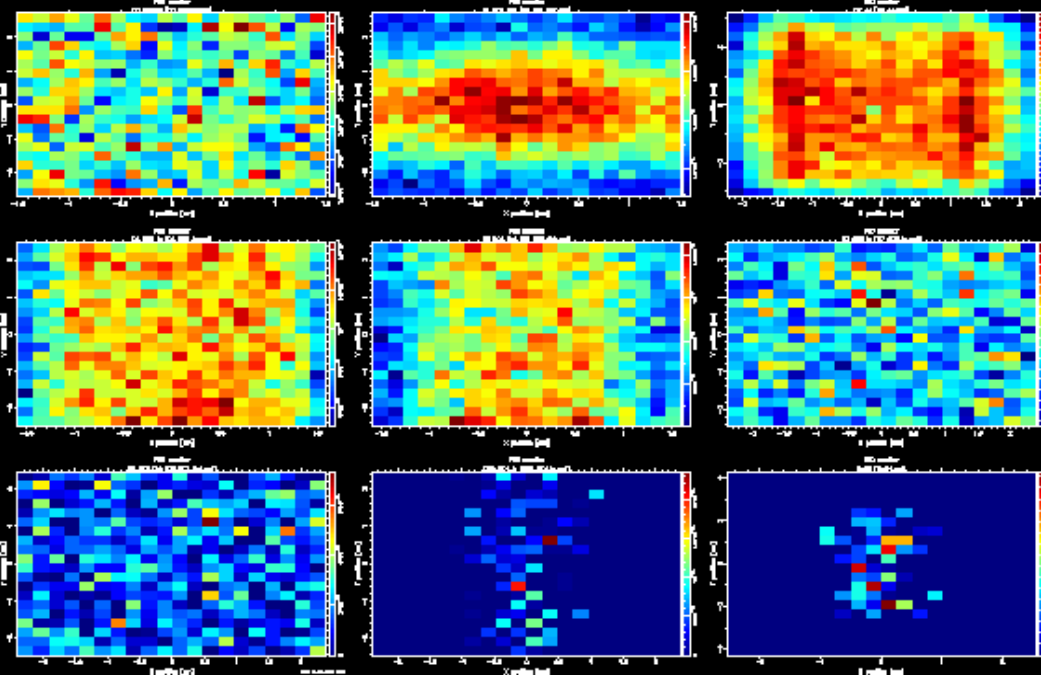Source_Optimizer ...
Source_simple ...
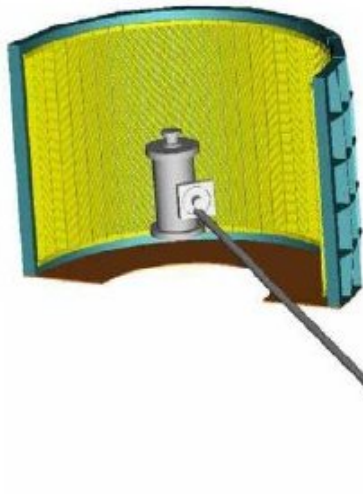Virtual_input ...
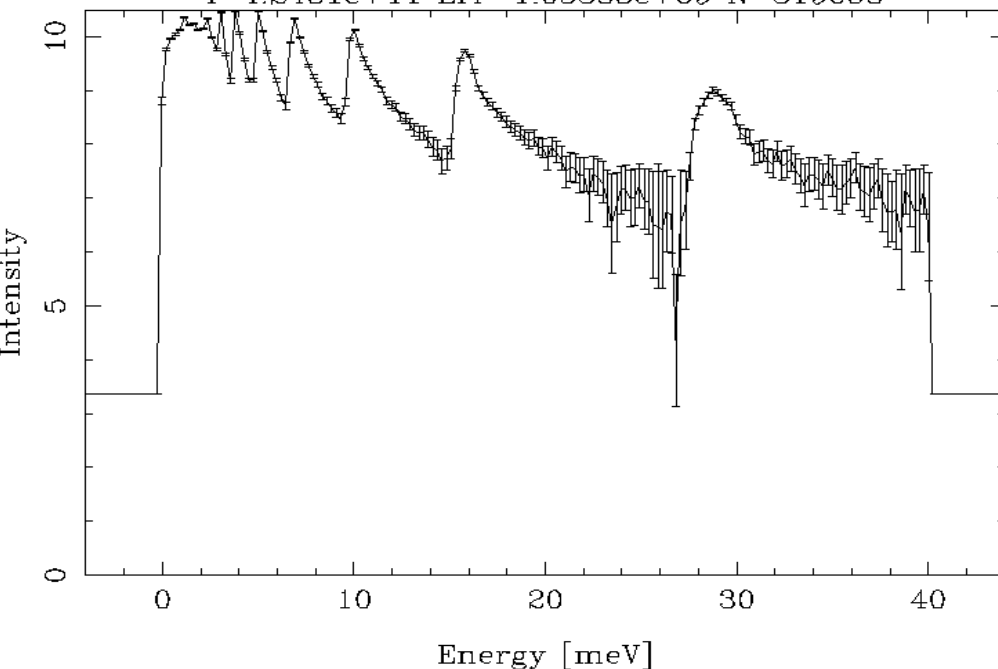Virtual_output ...

Line: 107 of 267 total, Column: 30

Time-Of-Flight (LET,ISIS)

McStas

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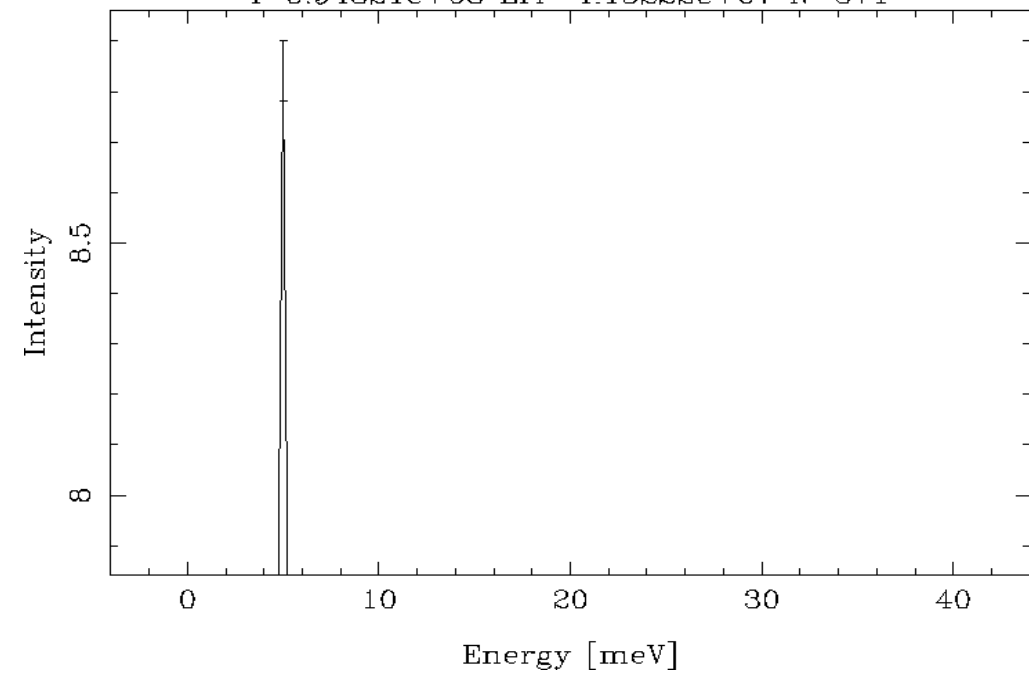- Subtle effects like of mismatch in chopper/guide geometry simulated (right)

PSD_Res2_t1 [PSD_res2_t1.sim]
X0=0.014589; dX=0.475515; Y0=1.27039; dY=1.2142;
I=1.96671e+06 Err=85275.4 N=1471

[LOG] E_mon_after_Res1 [rerun3/E_mon_after_Res1.sim]
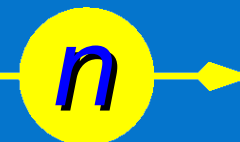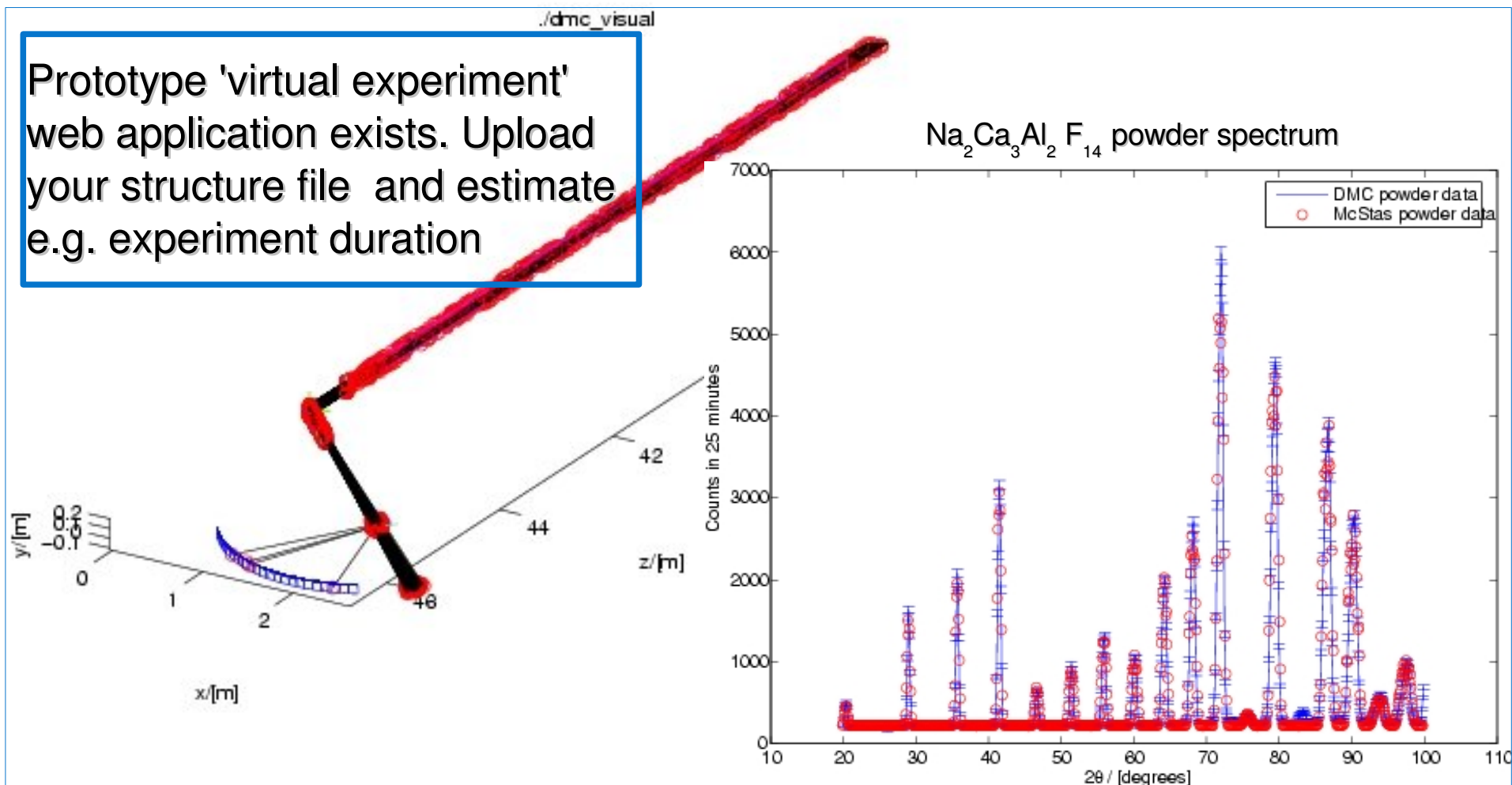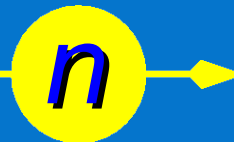X0=5.33633; dX=5.18527;
I=4.2431e+11 Err=1.05383e+09 N=319058
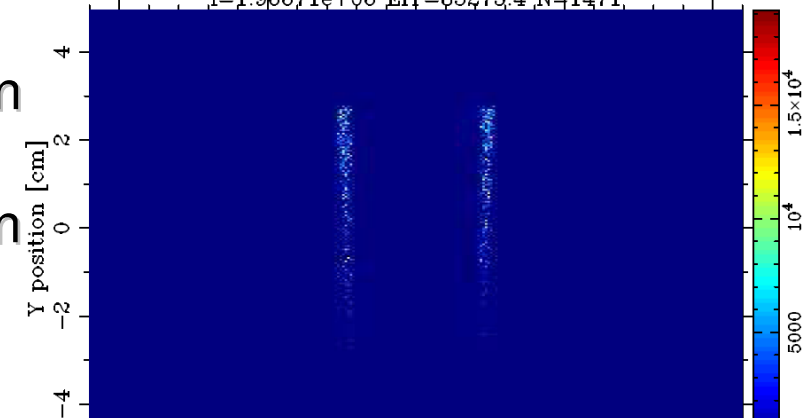
[LOG] E_mon_after_Res2 [rerun3/E_mon_after_Res2.sim]
X0=5; dX=0;
I=6.94321e+08 Err=4.15222e+07 N=571

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

./dmc_visual

$Na_2Ca_3Al_2F_{14}$ powder spectrum

- DMC powder data
- McStas powder data

Counts in 25 minutes
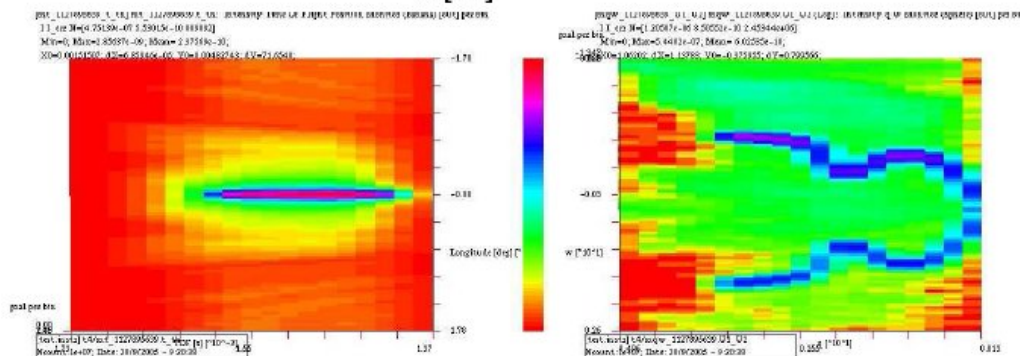
2θ / [degrees]
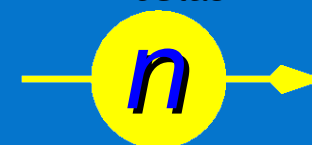
New – concentric comps
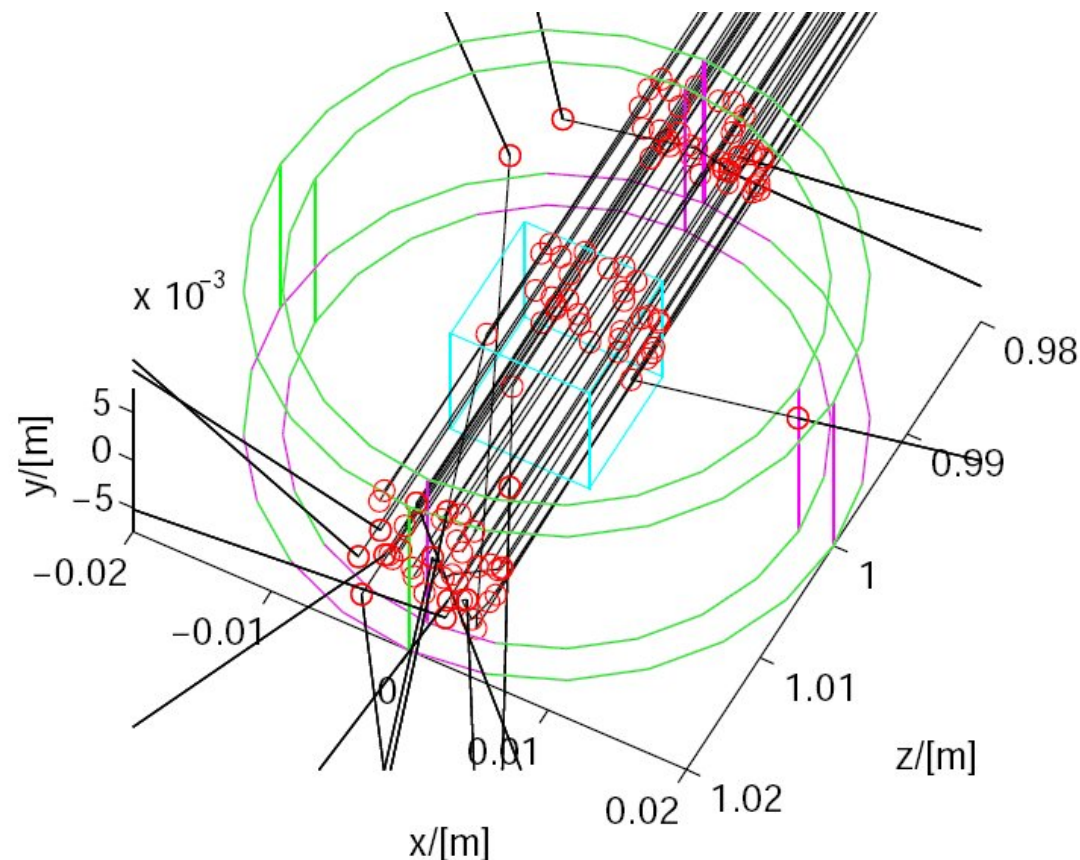
Components *inside* components.

Example: Liquid He (Isotropic_Sqw) inside Al Cryostat.

Al Powder lines separated from He rotons.

tract nº: HII3-CT-2003-

New – WHEN keyword

- *Mix* contributions from several scattering components
  - Phonon + Single crystal / ...
- Use to *parametrize* which sample component to use
  - Vanadium/Powder/Single crystal/...
- Use to *skip* certain parts of the instrument in certain configurations
  - With/without collimator

D7_SC3_In [D7_SC3_In.psd]
X0=0.283295; dX=2.75749; Y0=0.0156319; dY=1.29919;
I=3.37414e-11 Err=4.48959e-13 N=12875
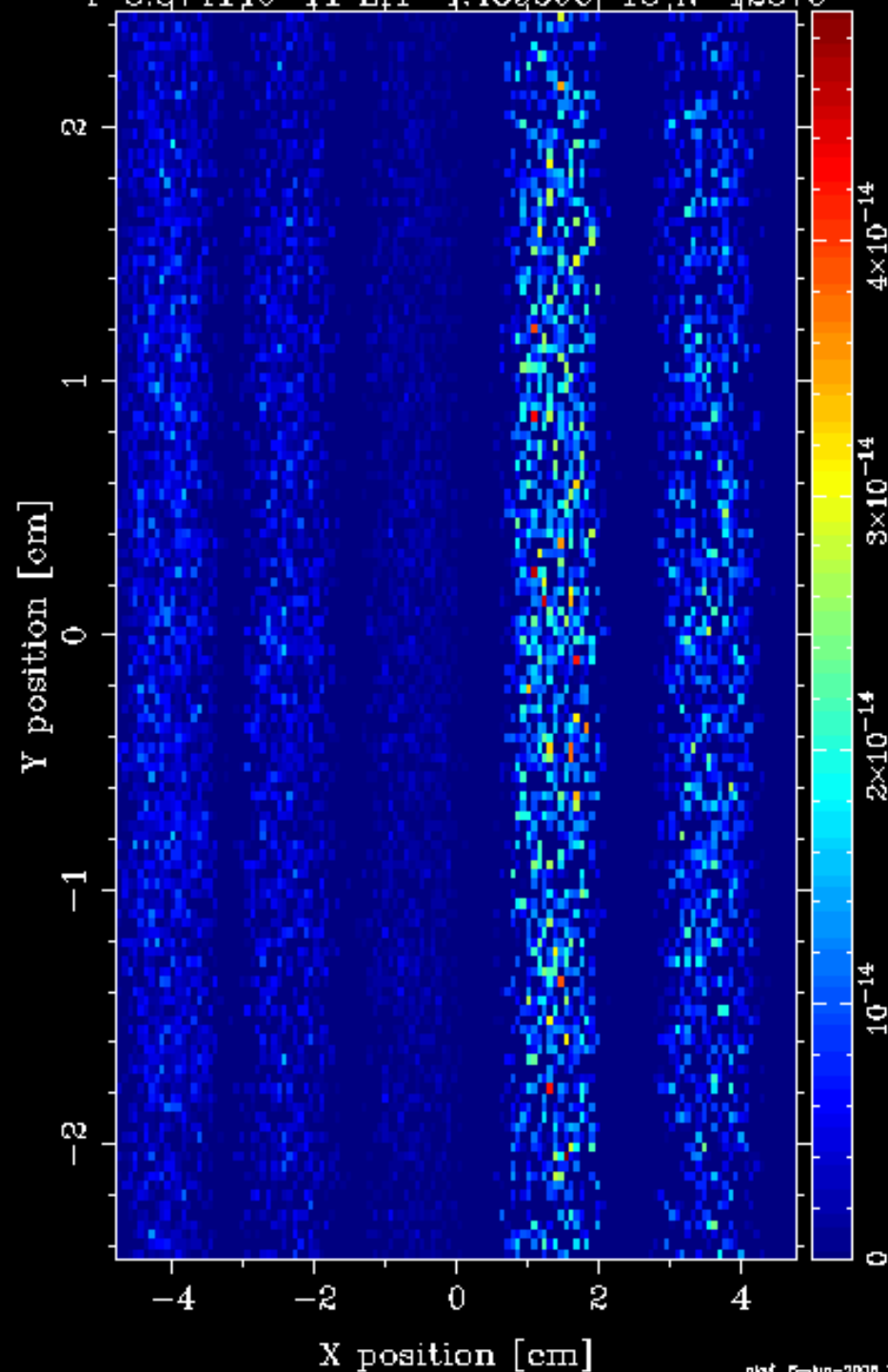
Lines [Lines_1148025579.x]
X0=0.00303455; dX=0.0275439;
I=4.43165e-11 Err=5.14841e-13 N=16943

plot 5-Jun-2006 14:38
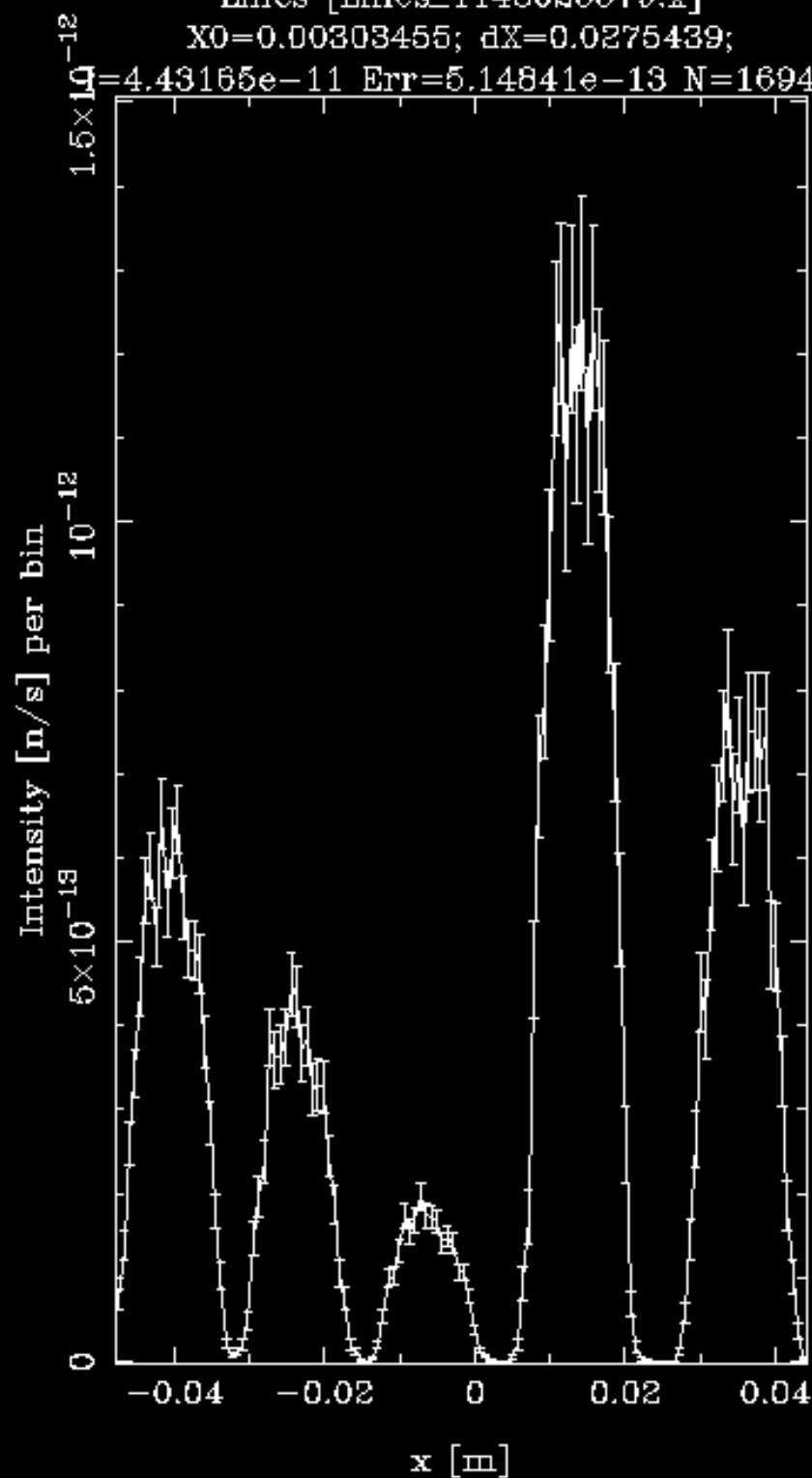
D7_SC3_ln [D7_SC3_ln.psd]
X0=0.0597546; dX=2.74726; Y0=0.0161714; dY=1.39802;
I=3.01641e−11 Err=3.18116e−13 N=15364
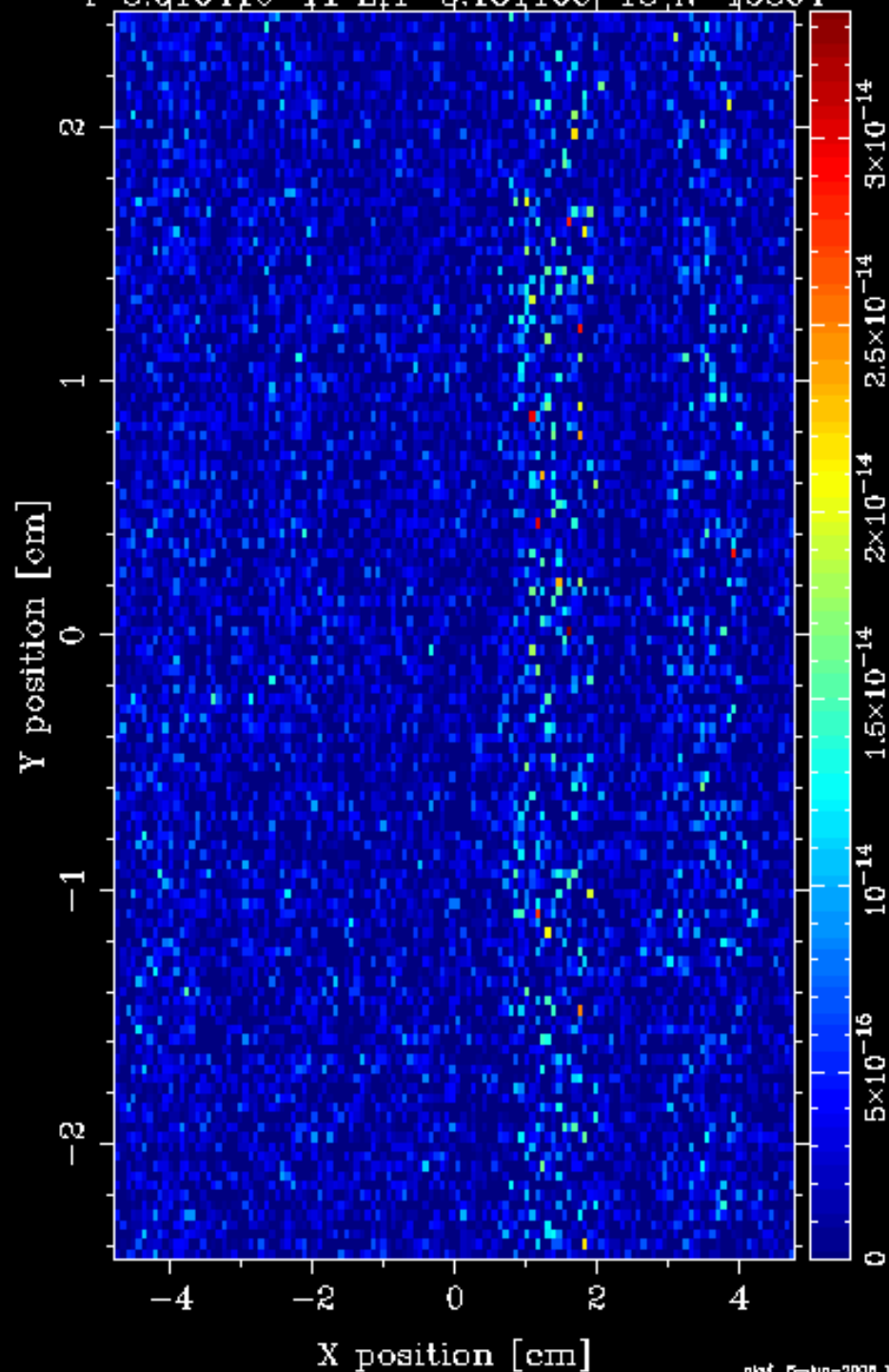
Lines [Lines_1148025702.x]
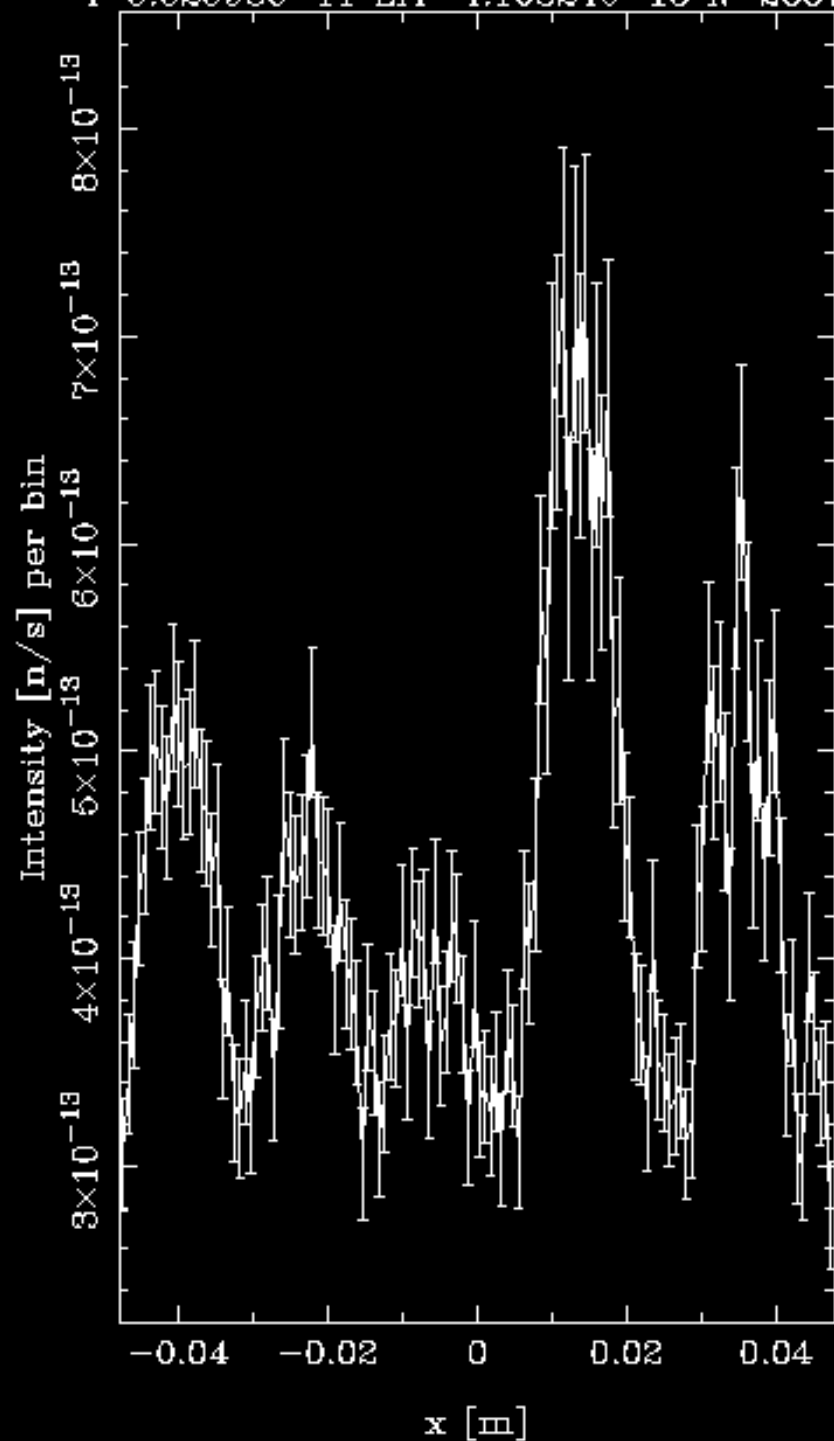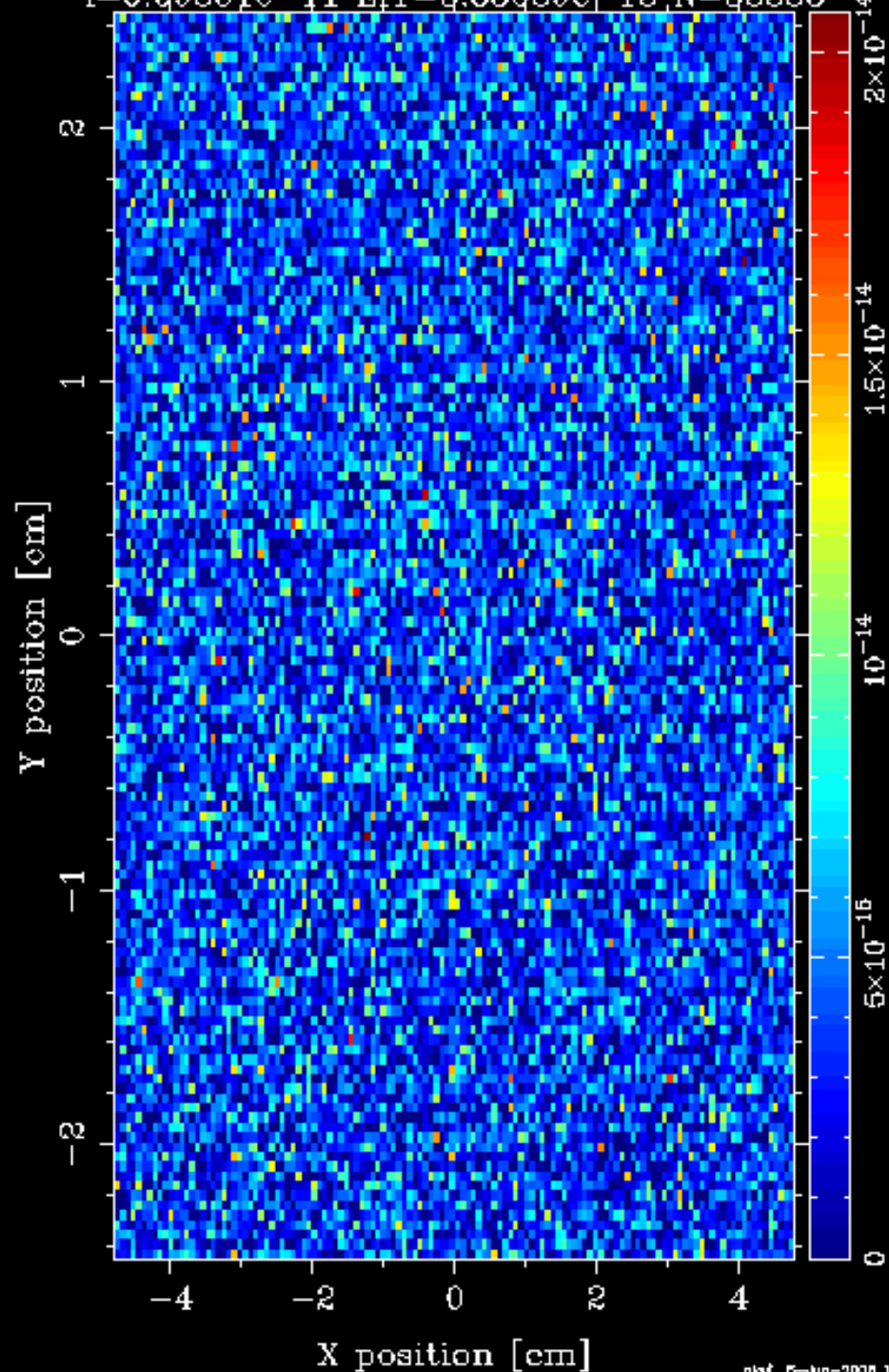X0=0.000511493; dX=0.0273964;
I=5.52598e−11 Err=4.16824e−13 N=28873

pkvf 6-Jun-2006 14:39

D7_SC3_In [D7_SC3_In.psd]
X0=−0.0172499; dX=2.7395; Y0=0.0197249; dY=1.40621;
I=6.09851e−11 Err=3.83689e−13 N=33388

Lines [Lines_1148025787.x]
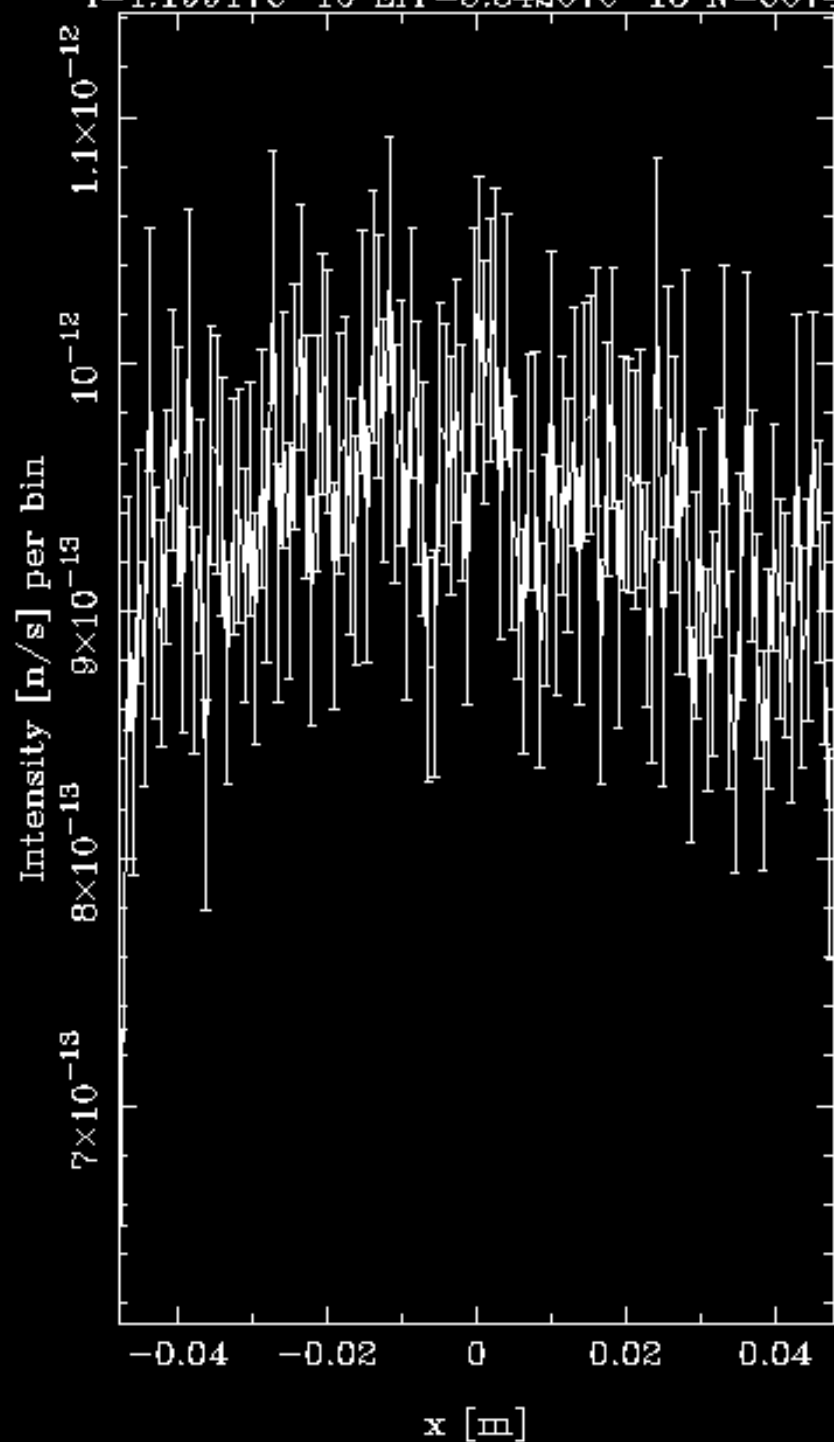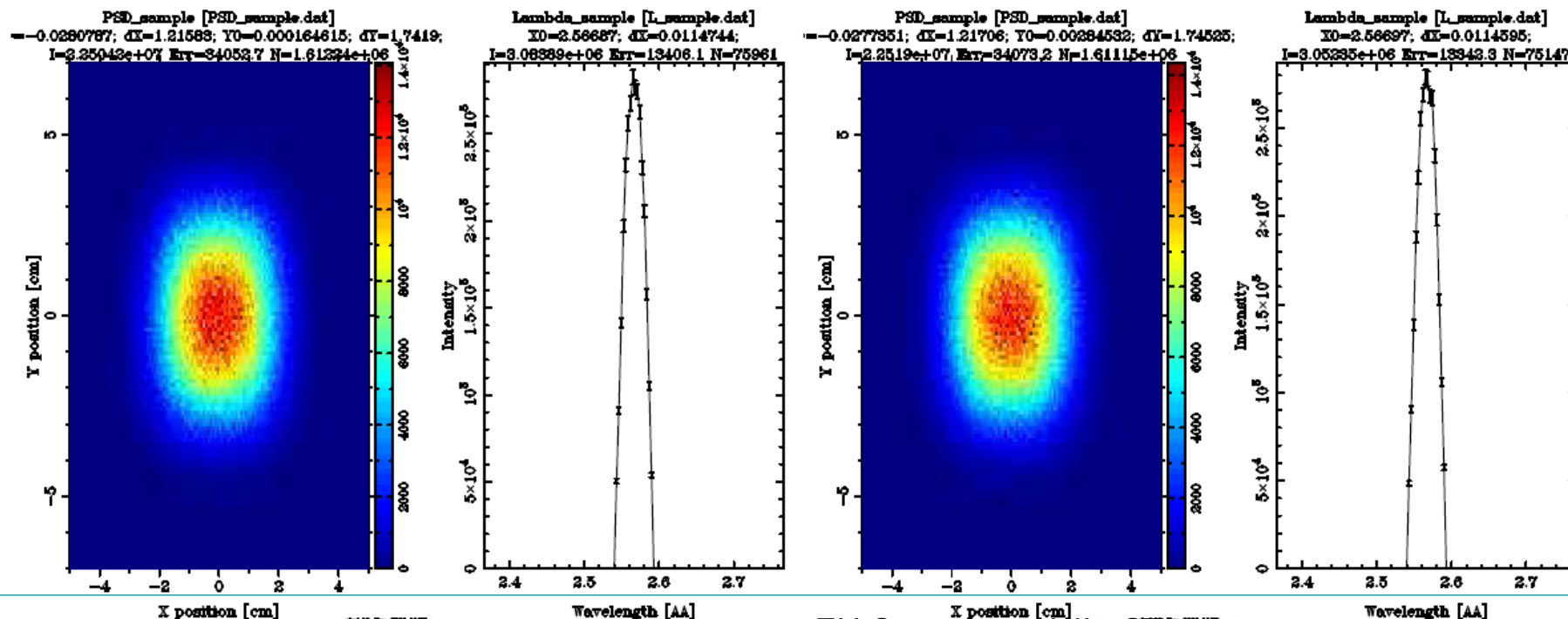X0=−0.000149018; dX=0.0272566;
I=1.19917e−10 Err=5.34267e−13 N=66741
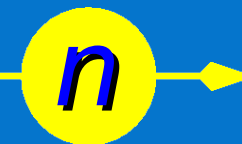
New – JUMP keyword

- Use to *teleport* to component
- *Iterate* a given component

Example: 49 versus 1 guide element for curved guide desc.

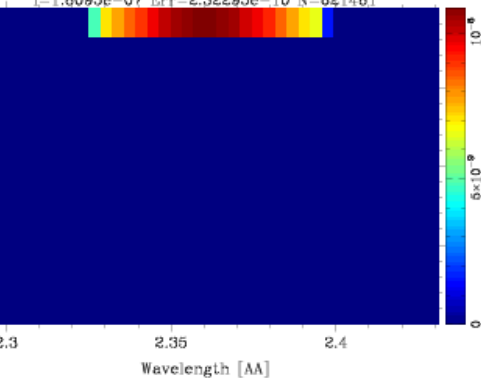473 (29064) vs. 196 (11481) lines of instr (c)code.

Polarisation support added

- ## First basic components added:
  - ### Spin flipper
  - ### Spin direction monitors
  - ### Vanadium with spin flip amplitudes
- ## More to come:
  - ### Peter Christiansen (Post Doc) recently hired for the purpose (Funding from ISIS TS2)
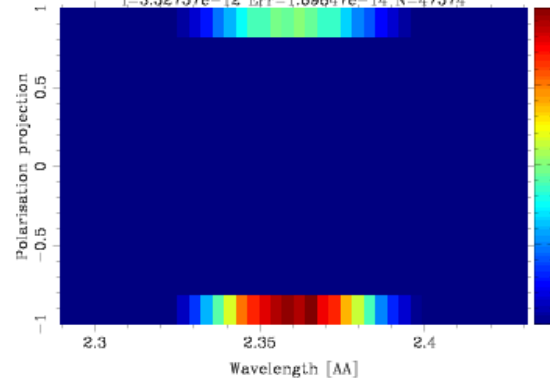 - ### Hiring again in the near future, will announce at neutron@anl.gov
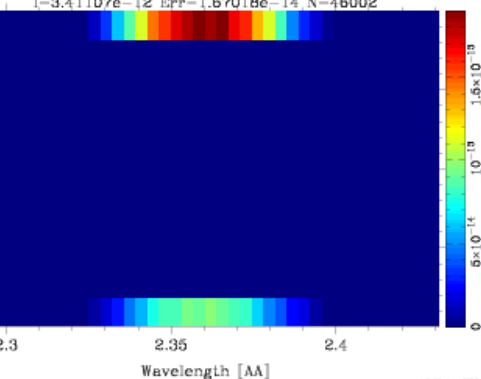
Polarisation support added
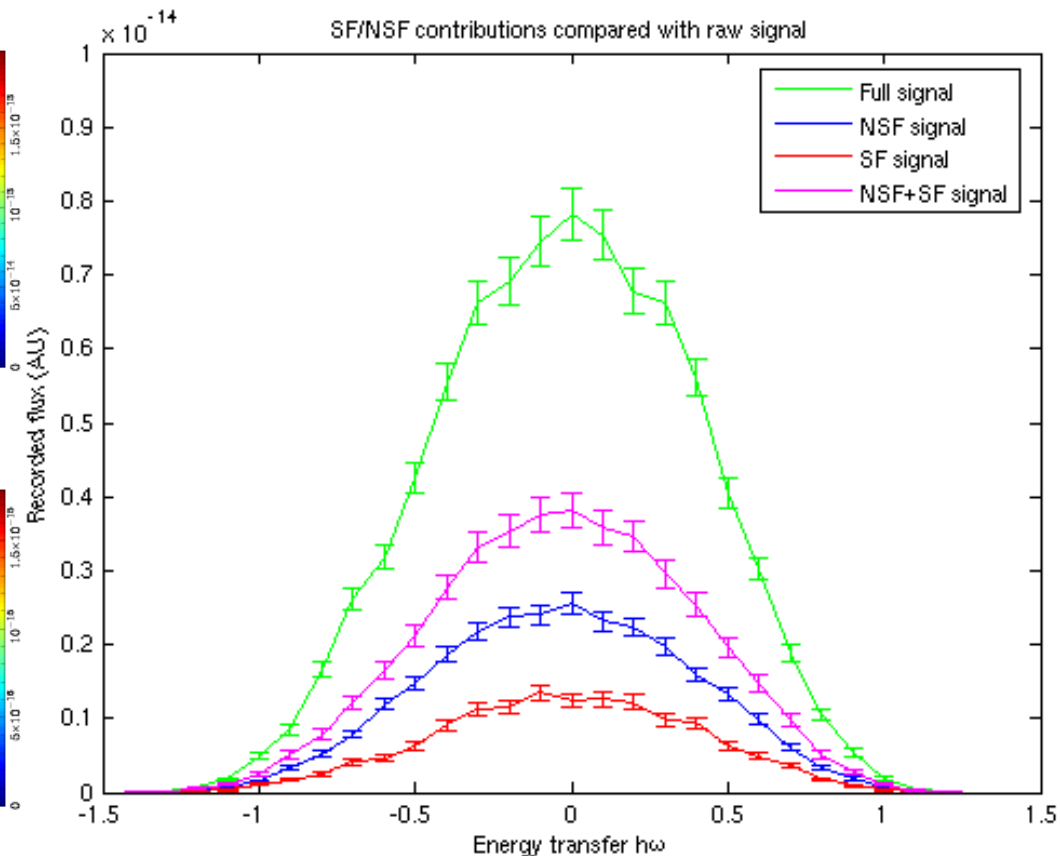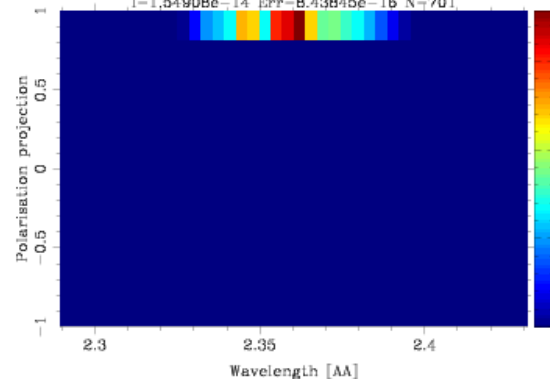
NEW TAS frontend template
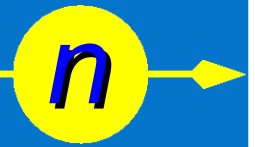
- Scan directly in reciprocal space, $\hbar\omega$ etc.
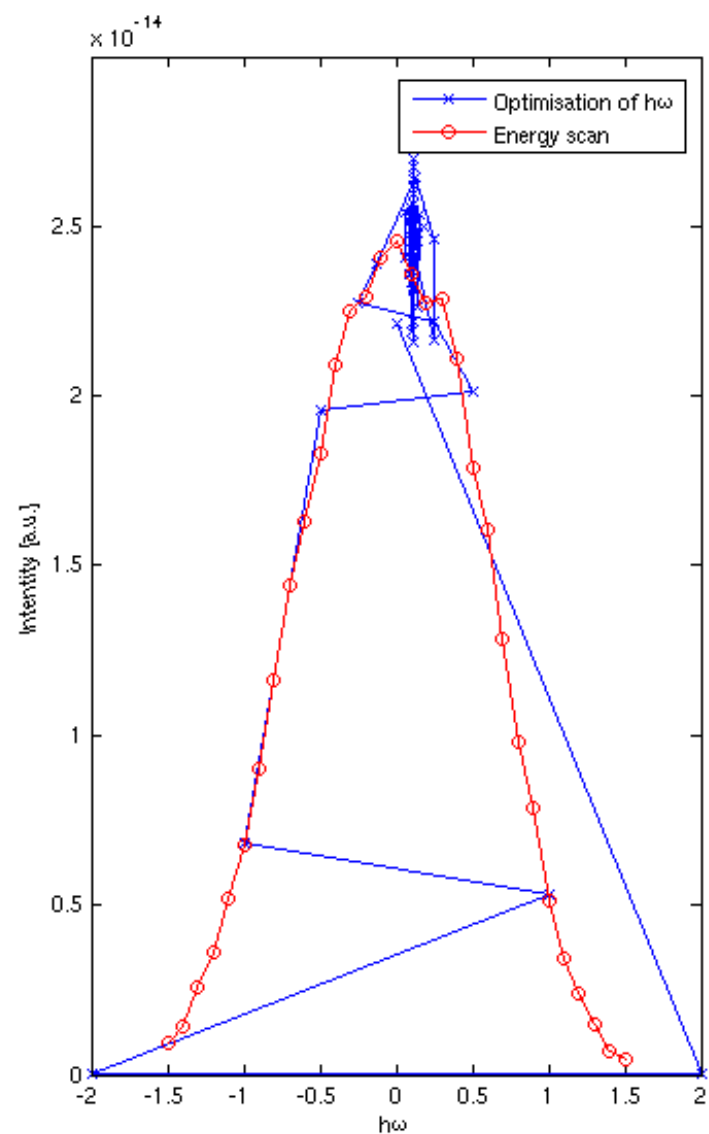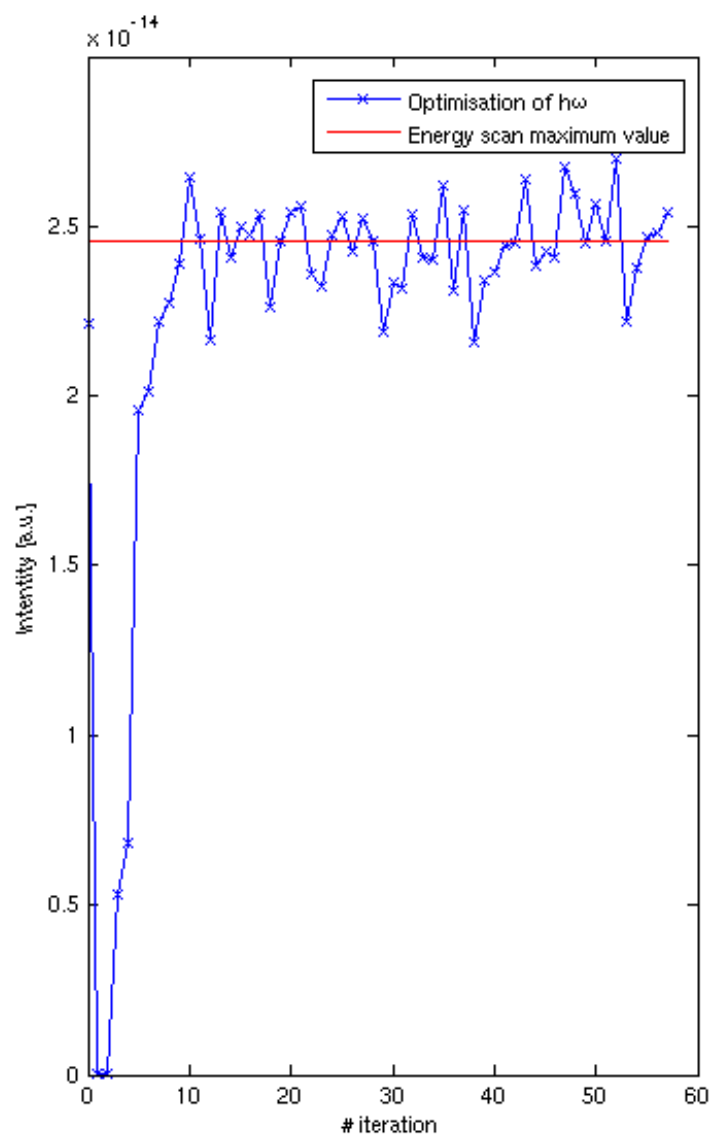- Tested ILL Tasmad code
- Currently ILL IN20 (configurable), more will follow
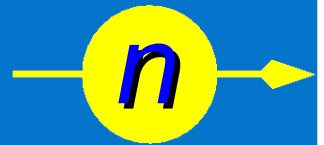- Easy resolution function calculation using Res_Sample

Optimisation support

Release date

- Planned release date of McStas 1.10 in September 2006

- Subscribe to neutron-mc@risoe.dk to stay informed (see http://www.mcstas.org)

The future

- Foresee increased work on components

- Emphasis on testing/validation using theory/data

- Virtual experiments

- Virtual neutron school

- Plan to seek funding for parallel effort in X-ray scattering (ESRF + Copenhagen Univ. interest)
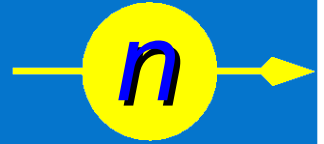
Funding

- Currently in EU FP6 (NMI3-MCNSI JRA):

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

- Hope to be in FP7 as well.
- Non-EU contributions (manpower, funding etc.) very welcome.

Conclusion

- McStas is / has
    - User-friendly, multi-platform, mature
    - TAS, TOF, DIFF, SANS, ...
    - Many sample models
- With the new keywords you can have:
    - Realistic samples with sample environment description
    - Easier description of curved guide systems / complex geometries
- Next release (fall 2006) will also include:
    - First polarisation code (Long awaited!)
    - Reciprocal space calculator
    - Optimisation tool
    - Focus now on:
    - Testing / validation of existing components
    - Virtual experiments
- Future:
    - Possibly X-ray 'sister-package'