

McStas 1.10

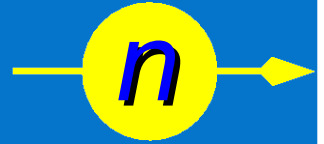
*new release of the flexible neutron ray-tracing package -
improved support for virtual experiments*

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Agenda

- 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
<http://www.mcstas.org>

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

Short McStas introduction



- Users at major labs



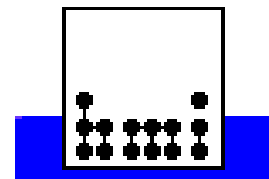
NIST



PAUL SCHERRER INSTITUT
PSI



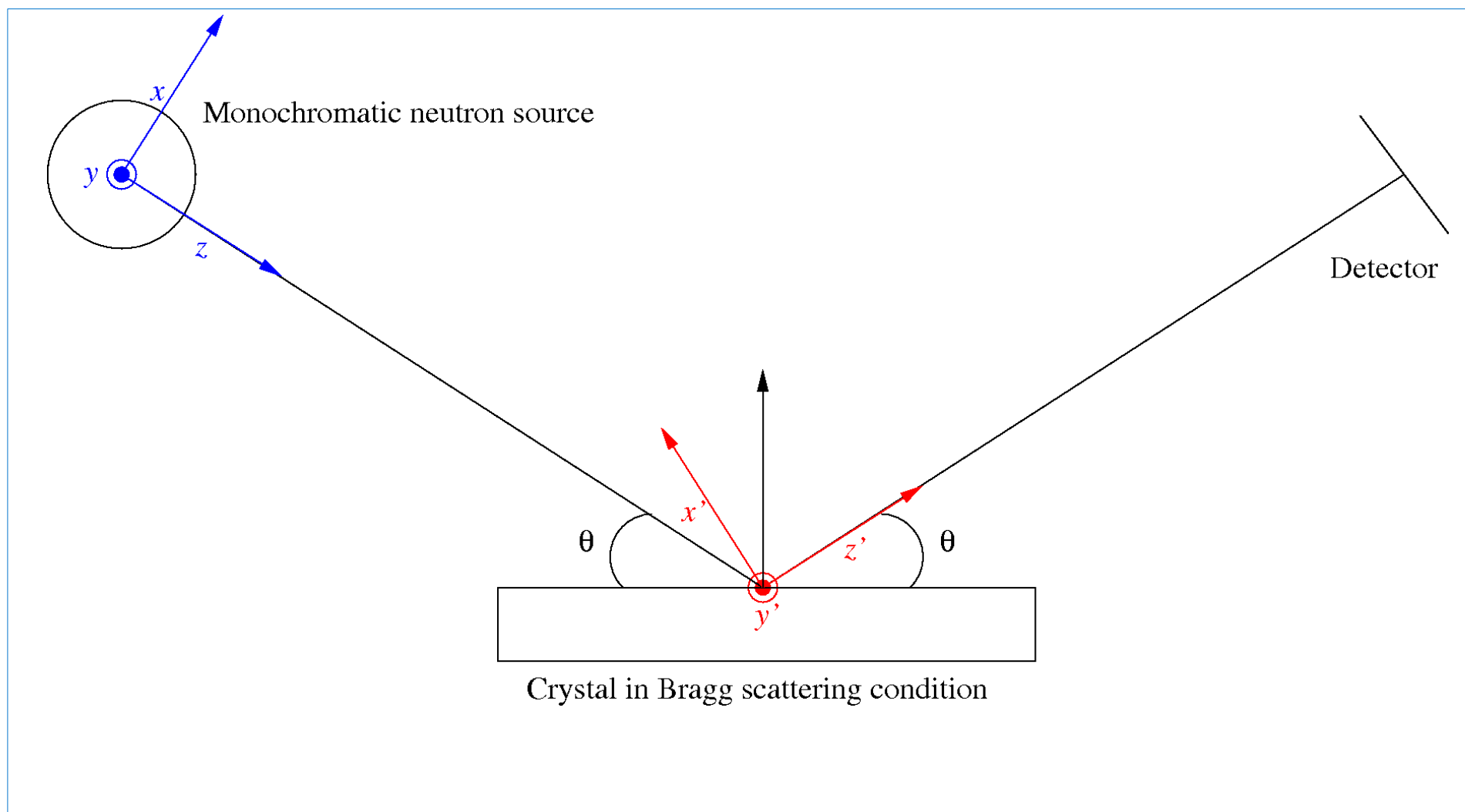
Forschungszentrum Jülich
in der Helmholtz-Gemeinschaft



JAEA and KEK Joint Project



Short McStas introduction



Short McStas introduction



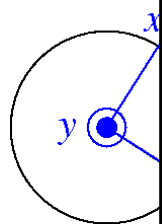
Neutron ray/package:

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

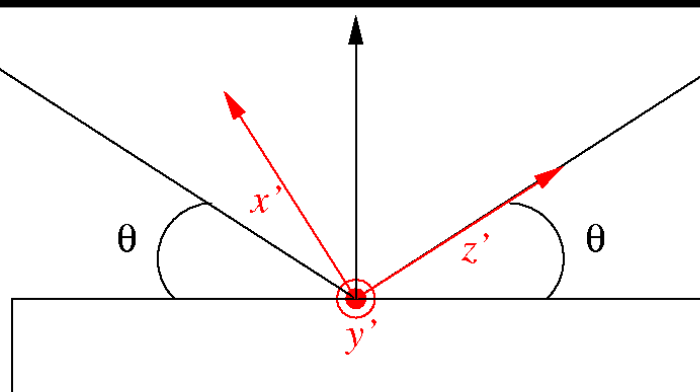
Coordinates (x, y, z)

Velocity (v_x, v_y, v_z)

Spin (s_x, s_y, s_z)



ector

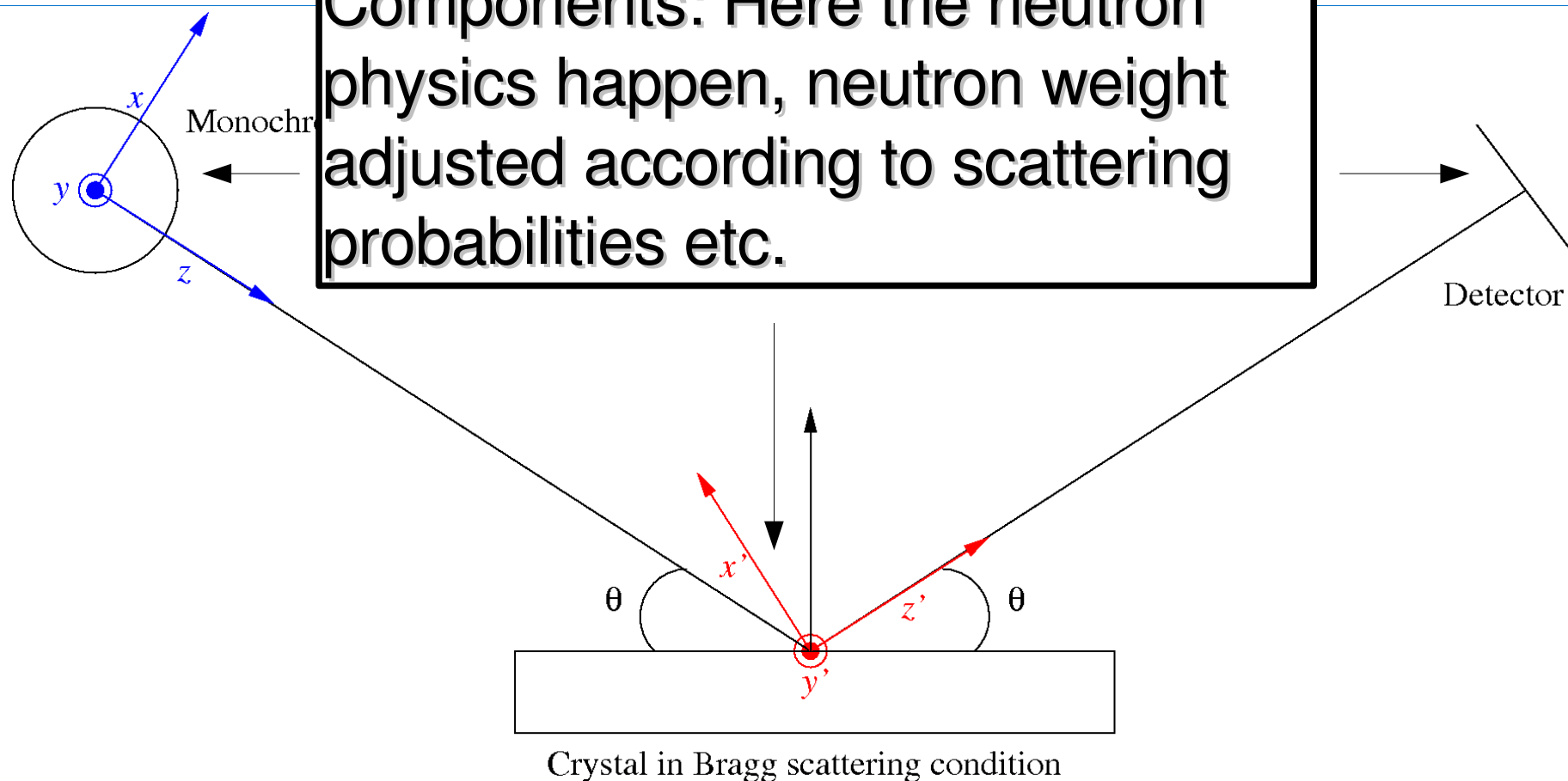


Crystal in Bragg scattering condition

Short McStas introduction



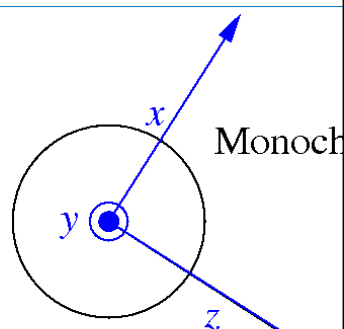
Components: Here the neutron physics happen, neutron weight adjusted according to scattering probabilities etc.



Short McStas introduction

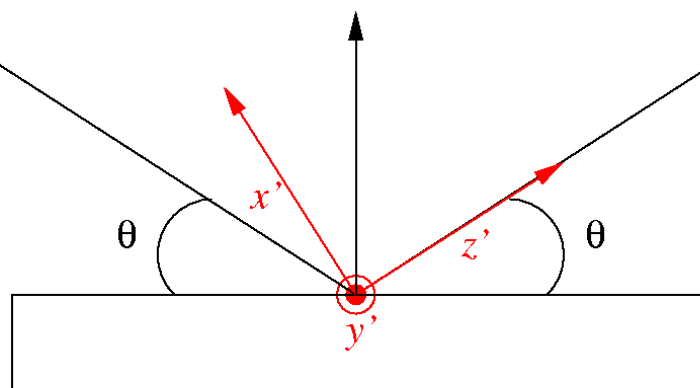


Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.



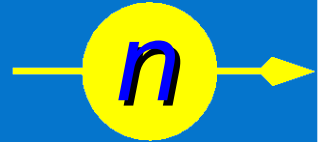
Monoch

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

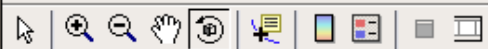
File Simulation Neutron site

Help (McDoc)

Insert Tools Desktop Window Help

Instrument file: h8_test.instr

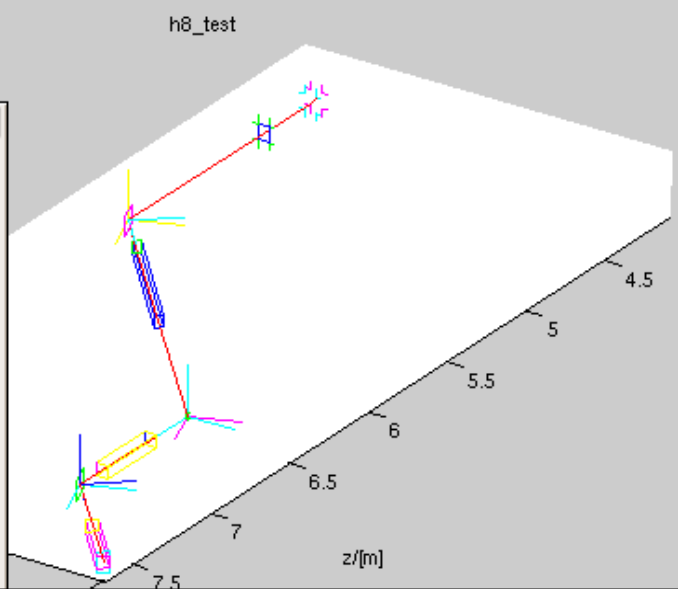
Edit/New Run



Simulation results: mcstas.sim

Read Plot

Status: Done



Monochromator : (DM = 3.3539)
A1 = 20.60, A2 = 41.20
Ki = 2.662 Angs-1 Energy
Velocity = 1676 m/s, L
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=
SC3_In.psd"
Detector: D8_SC3_Out_I=
D8_SC3_Out.psd"
Detector: D10_SC4_In_I=
D10_SC4_In.psd"
Detector: He3H_I=2.3390
Simulation finished.
mcplot mcstas.sim
mcplot mcstas.sim

File Edit Search View

/* 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.
rx=20, ry=20, filename=
AT (0, 0, 0.0001) RELATIVE

/* SC1 collimator. 40'=3
COMPONENT SC1 = Guide(
w1 = 0.031, h1 = 0.054,

Line: 107 of 267 total, Column: 30

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

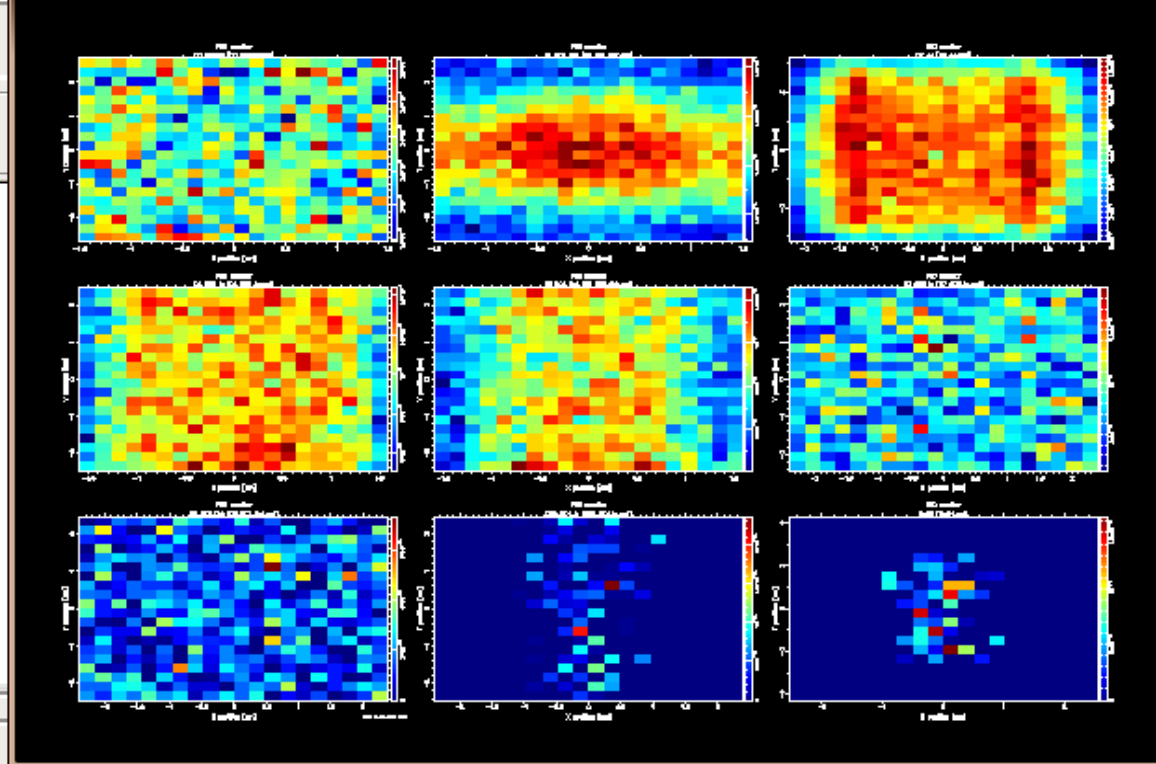
Last component:

Source
D0_Source

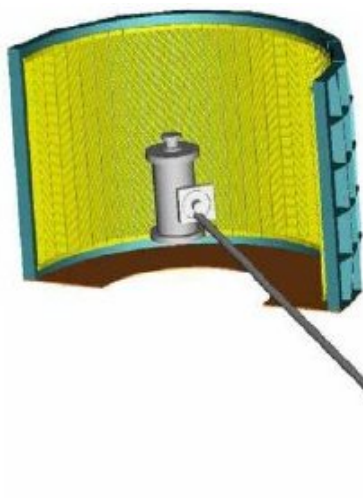
Start

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

PGPLOT Window 1

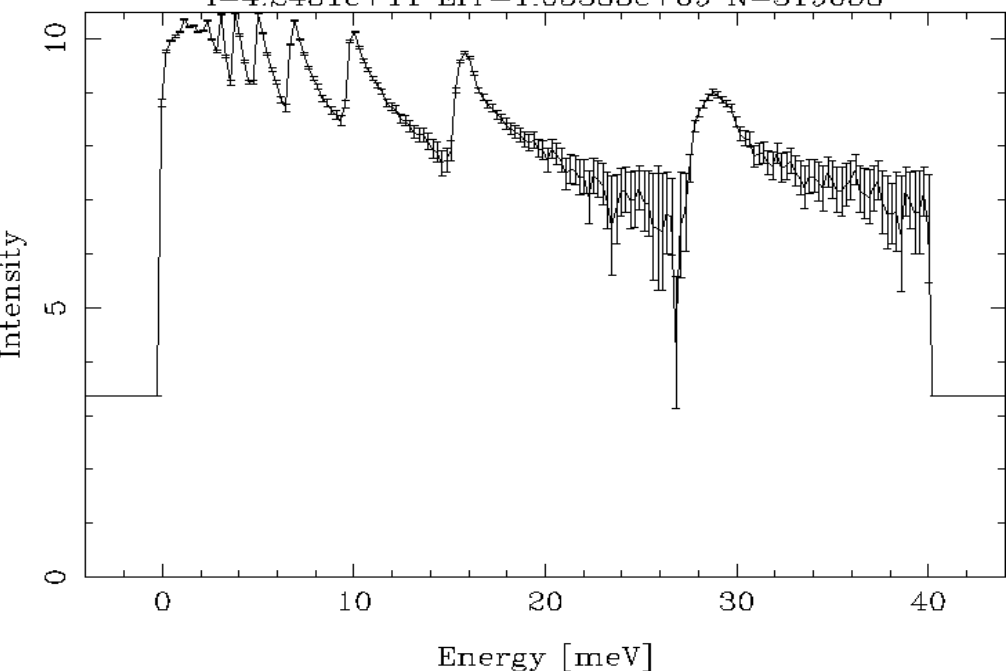


Time-Of-Flight (LET, ISIS)

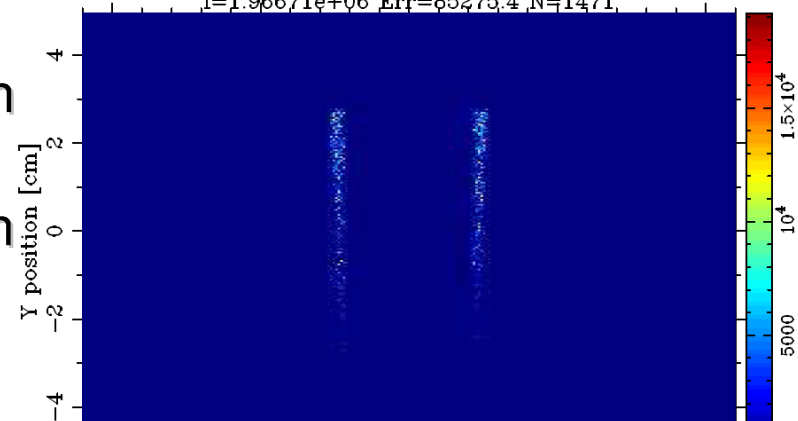


- Complicated design, total of 7 choppers!
- Notice effect of double resolution choppers below
- Subtle effects like of mismatch in chopper/guide geometry simulated (right)

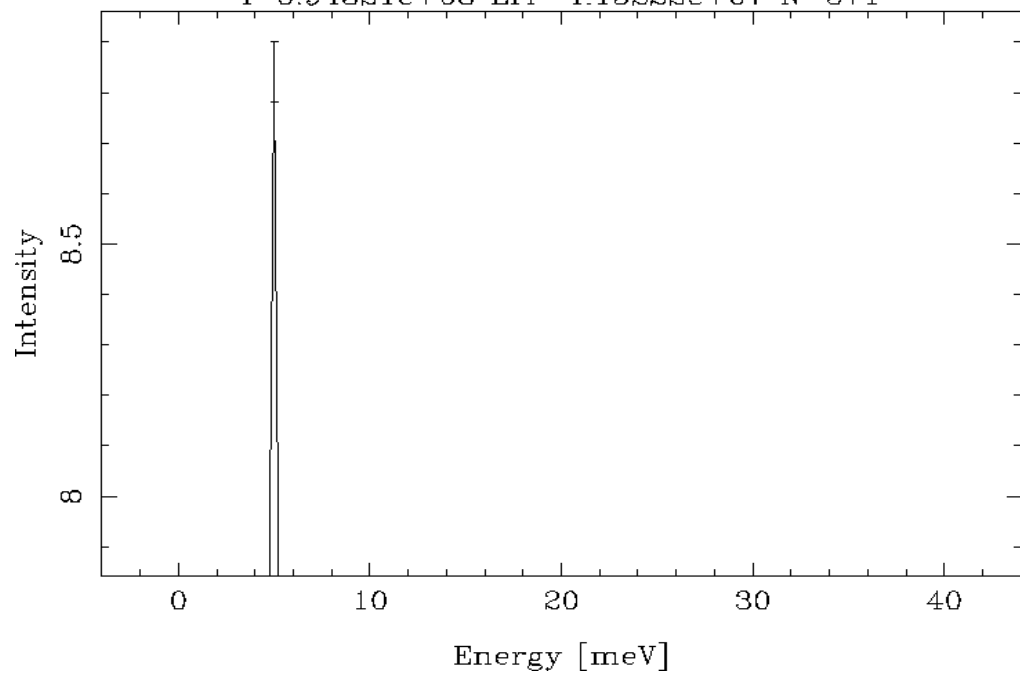
[LOG] E_mon_after_Res1 [rerun3/E_mon_after_Res1.sim]
 X0=5.33633; dX=5.18527;
 I=4.2431e+11 Err=1.05383e+09 N=319058



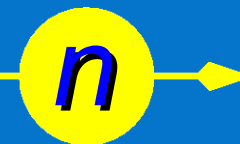
PSD_Res2_t1 [PSD_res2_t1.sim]
 X0=0.014589; dX=0.475515; Y0=1.27039; dY=1.2142;
 I=1.96671e+06 Err=85275.4 N=1471



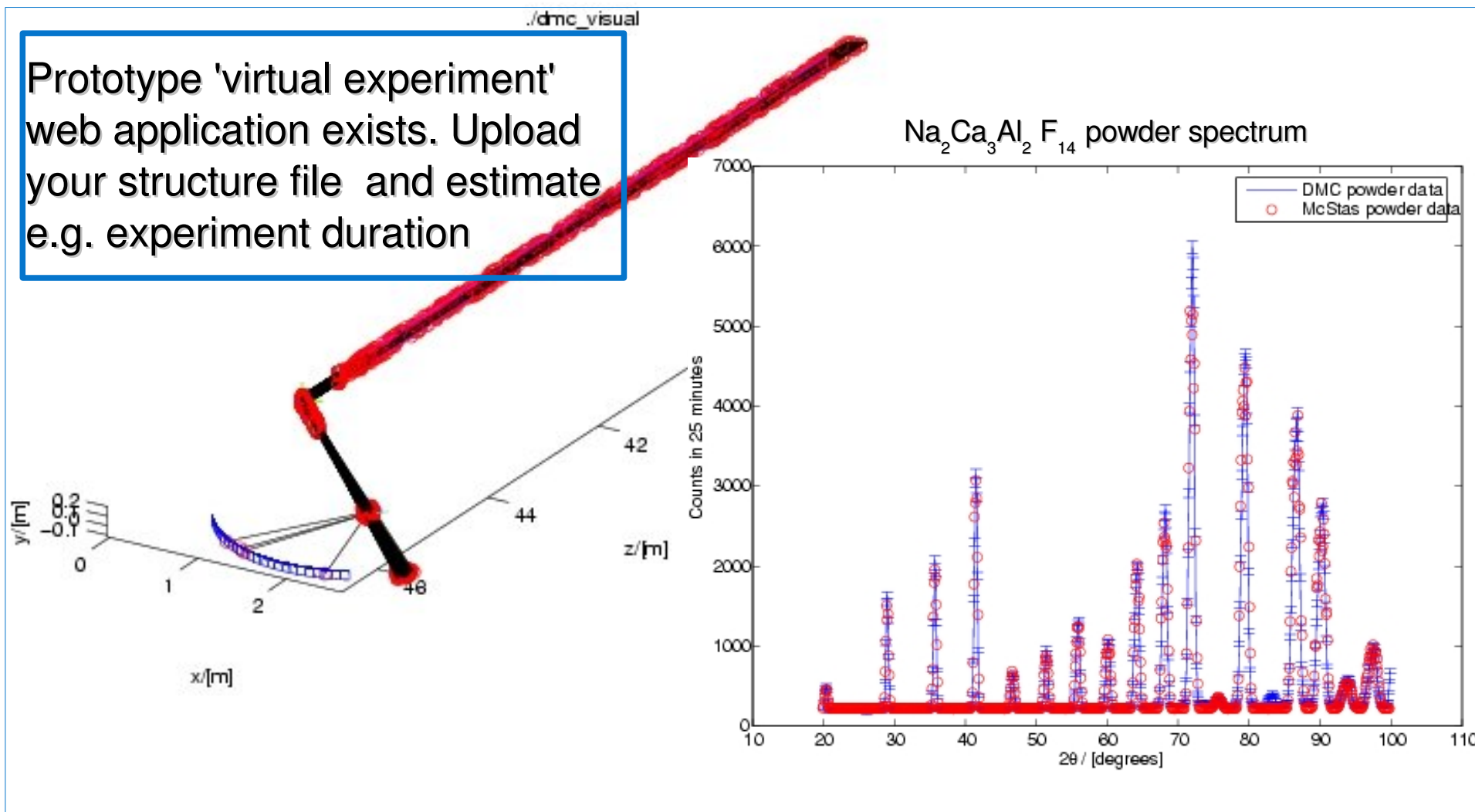
[LOG] E_mon_after_Res2 [rerun3/E_mon_after_Res2.sim]
 X0=5; dX=0;
 I=6.94321e+08 Err=4.15222e+07 N=571



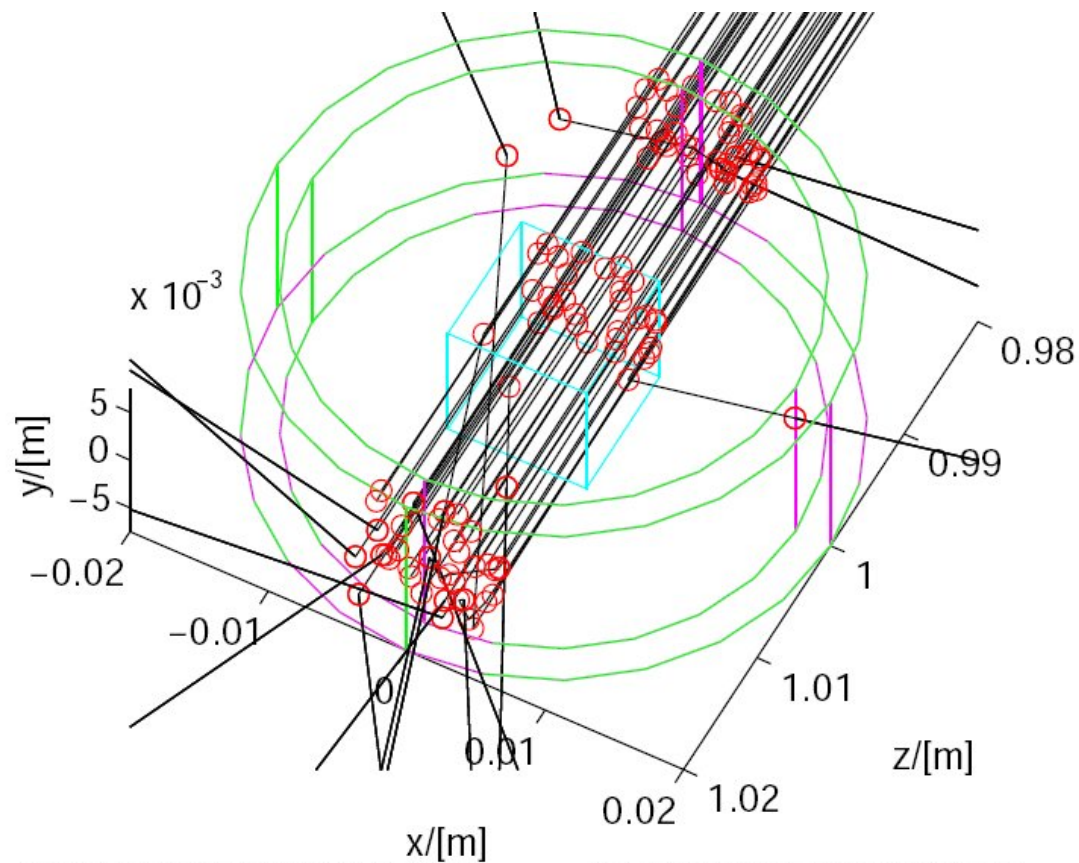
Powder Machine (DMC, PSI)



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



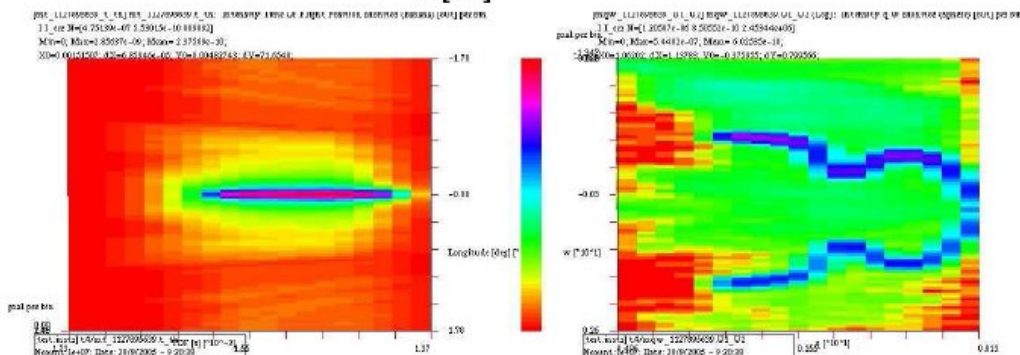
New – concentric comps



Components *inside* components.

Example: Liquid He (Isotropic_Sqw) inside Al Cryostat.

Al Powder lines separated from He rotons.



tract n^o: H13-CT-2003-



RISO



New – *WHEN* keyword

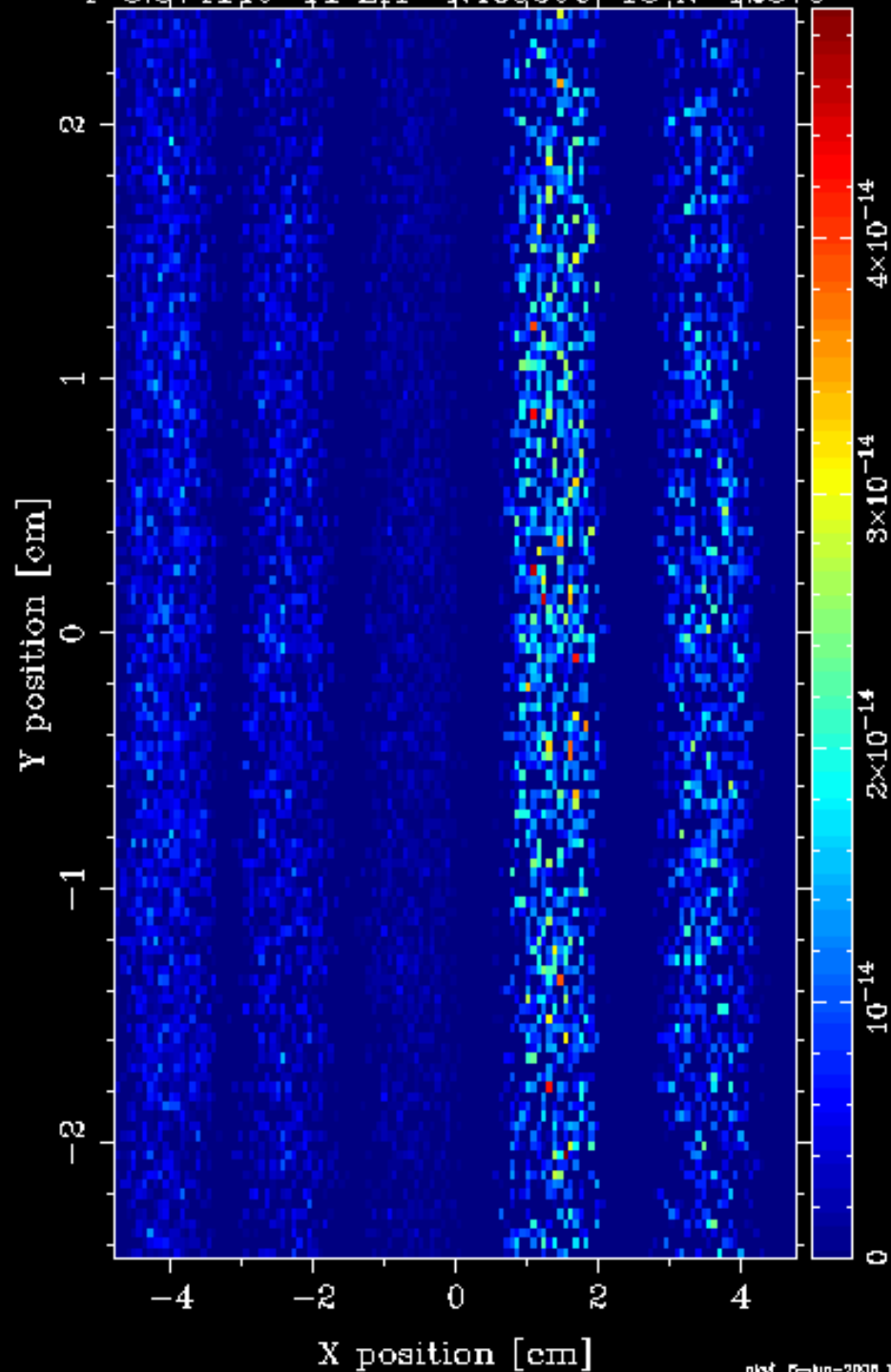
- *Mix* contributions from several scattering components
 - Phonon + Single crystal / ...
- Use to *parametrize* which sample component to use
 - Vanadium/Powder/Single crystal/...
- Use to *skip* certain parts of the instrument in certain configurations
 - With/without collimator



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

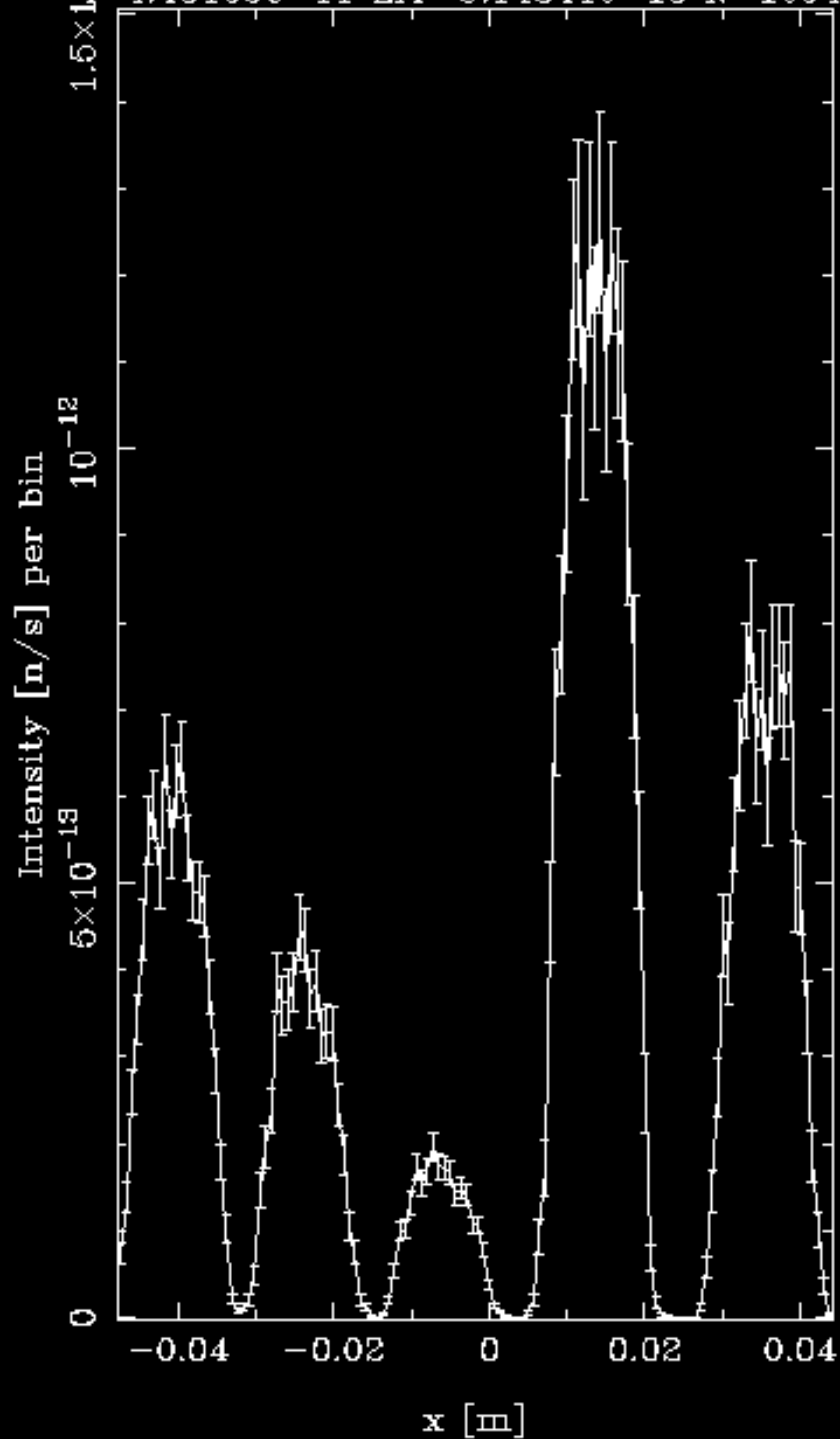


pkw 5-Jun-2000 14:39

Lines [Lines_1148025579.x]

X0=0.00303455; dX=0.0275439;

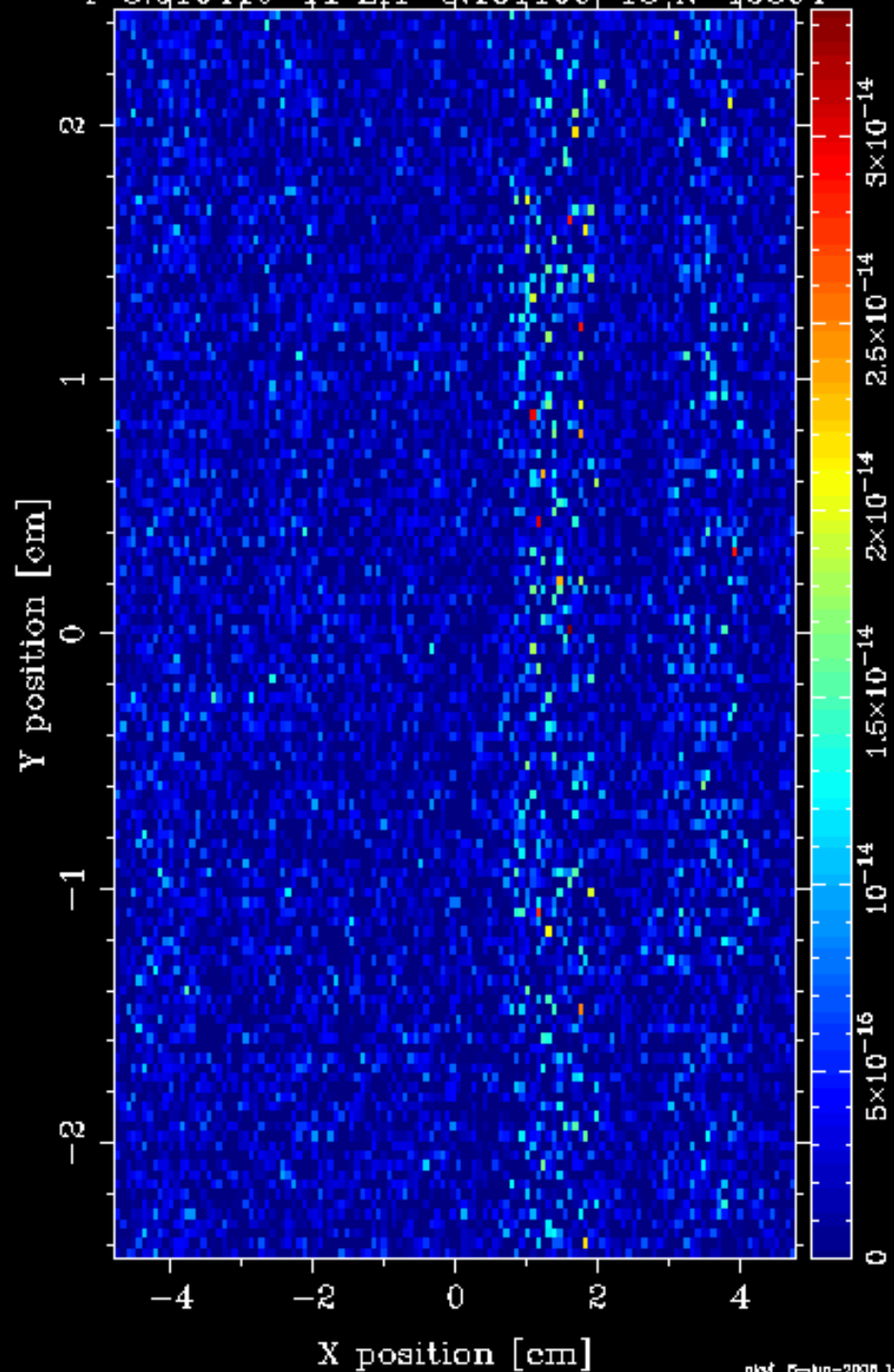
I=4.43165e-11 Err=5.14841e-13 N=16943



D7_SC3_In [D7_SC3_In.psd]

X0=0.0597546; dX=2.74726; Y0=0.0161714; dY=1.39802;

I=3.01641e-11 Err=3.18116e-13 N=15364

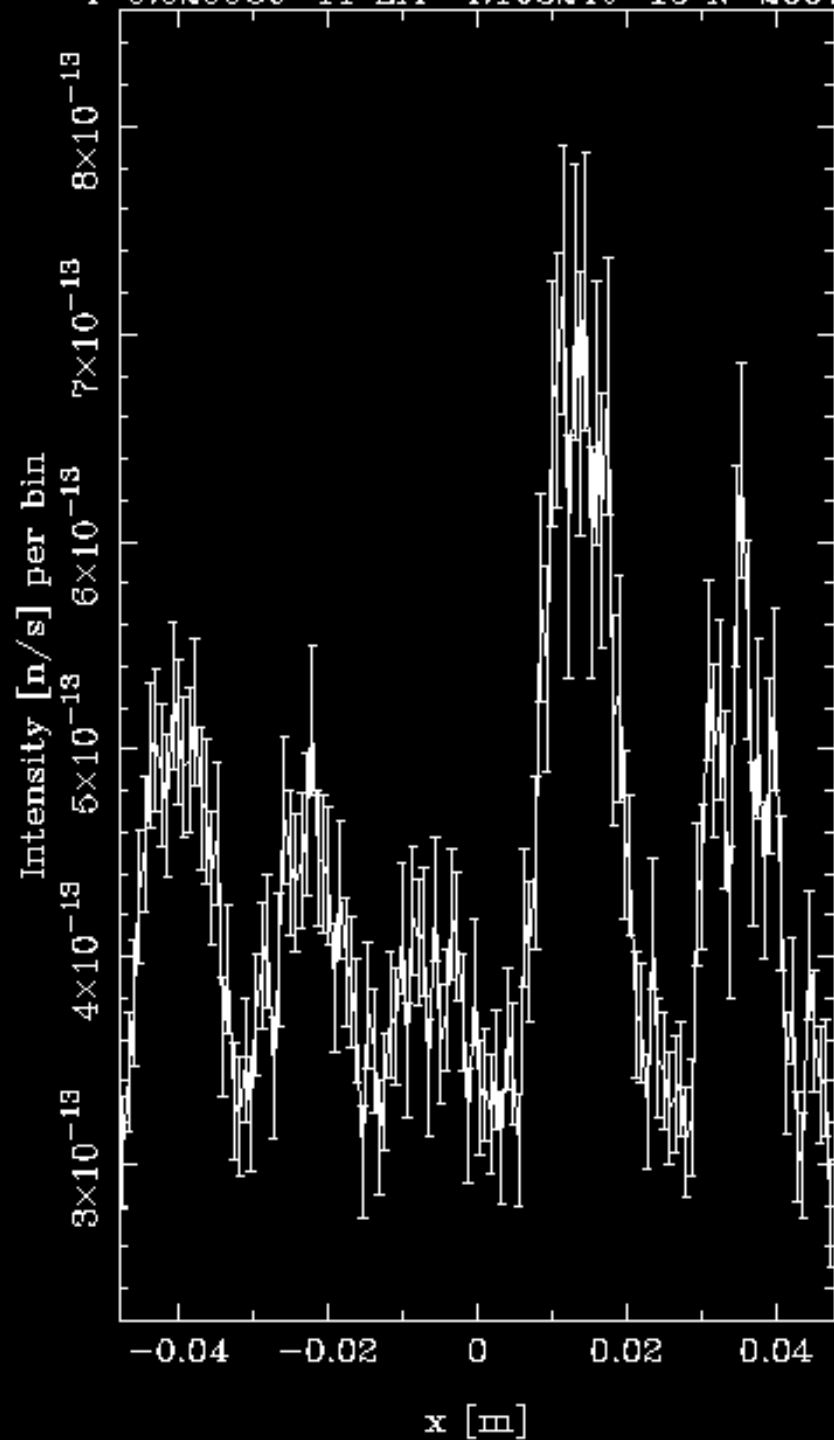


pkw 5-Jun-2000 14:39

Lines [Lines_1148025702.x]

X0=0.000511493; dX=0.0273964;

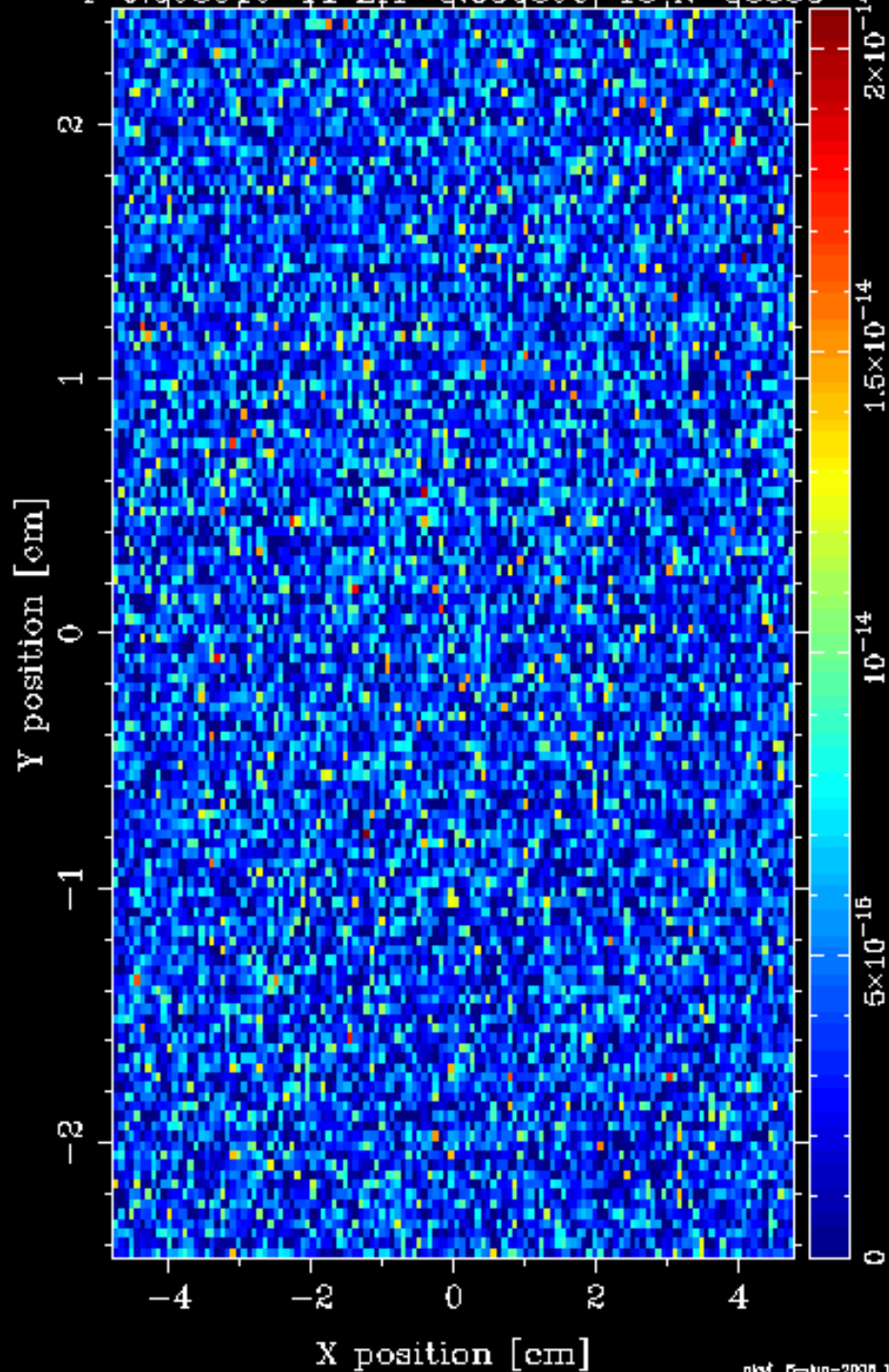
I=5.52598e-11 Err=4.16824e-13 N=28873



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

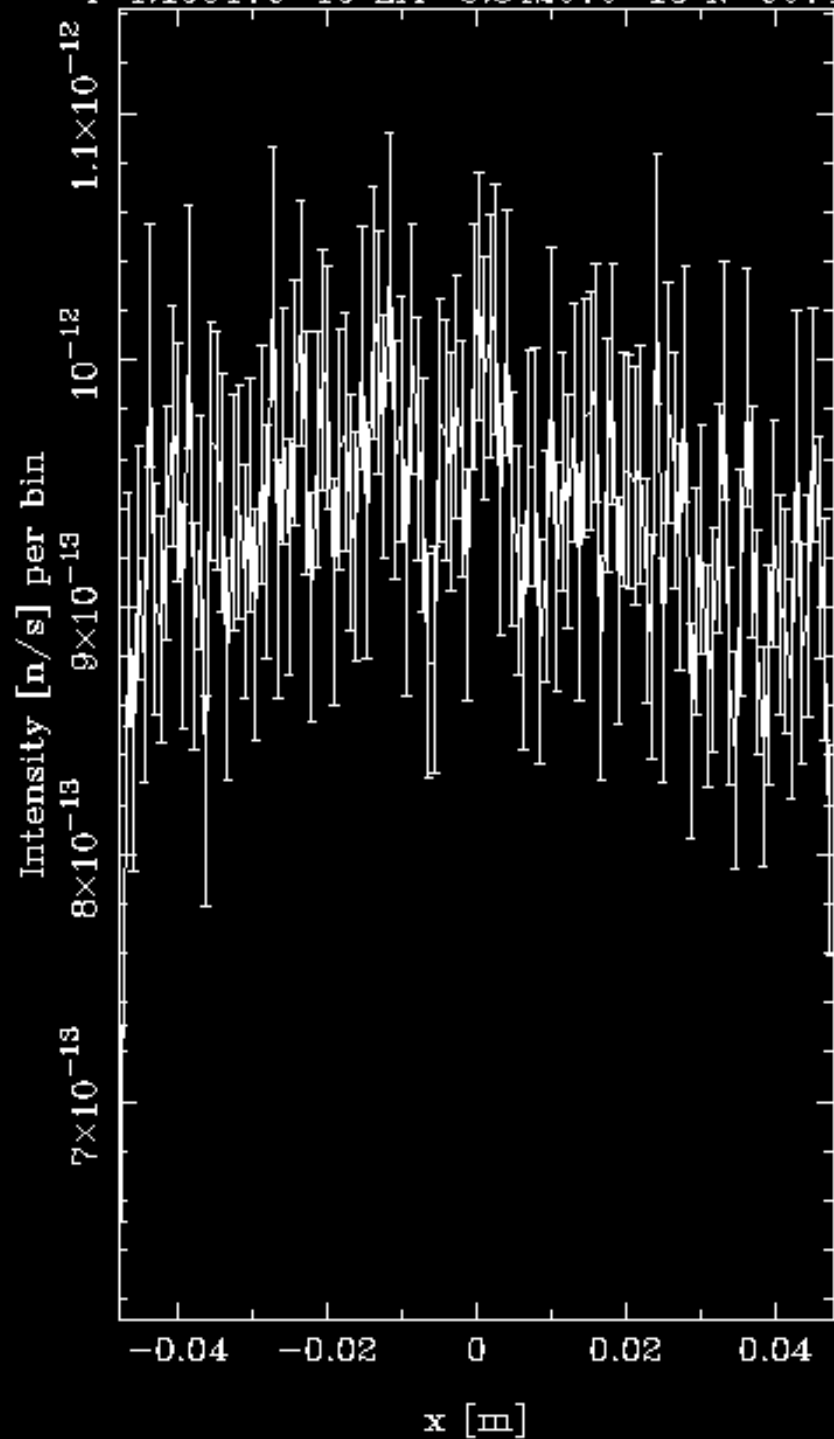


pkv 5-Jun-2000 14:39

Lines [Lines_1148025787.x]

X0=-0.000149018; dX=0.0272566;

I=1.19917e-10 Err=5.34267e-13 N=66741



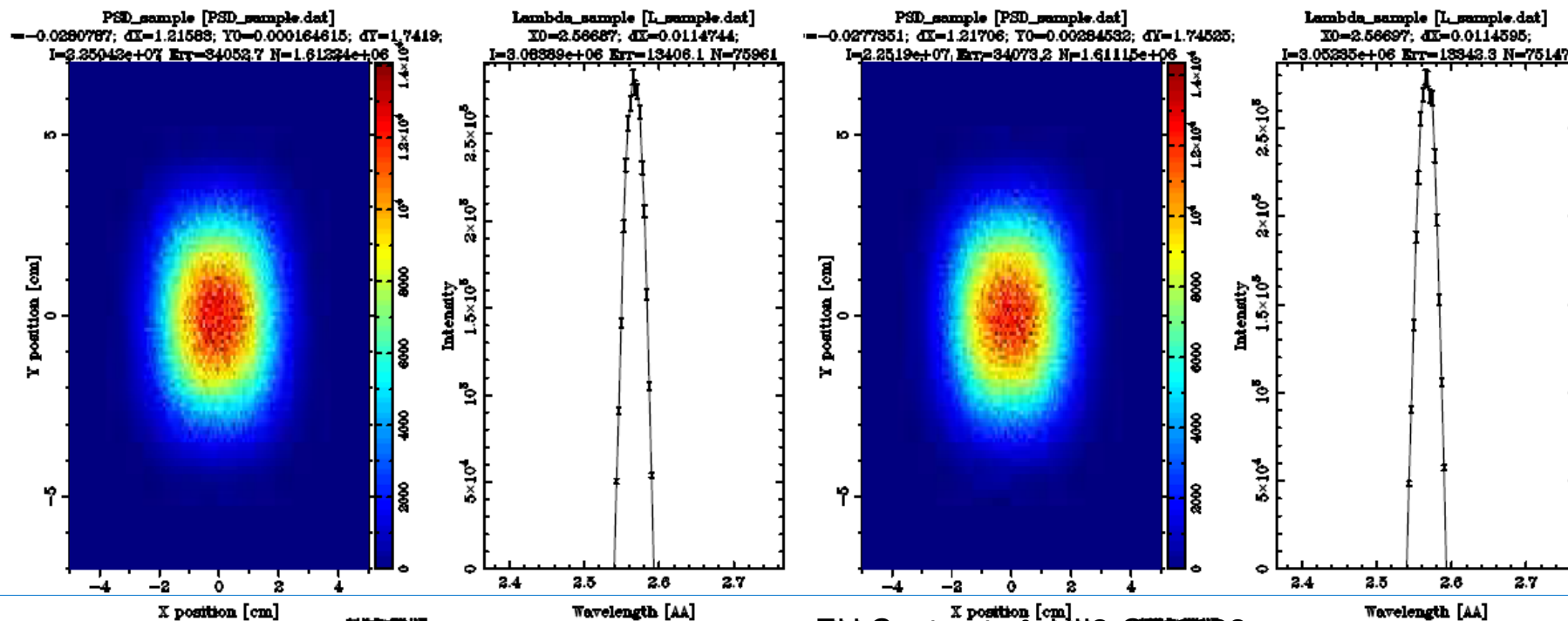
New – JUMP keyword



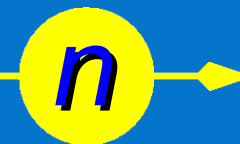
- Use to *teleport* to component
- *Iterate* a given component

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

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



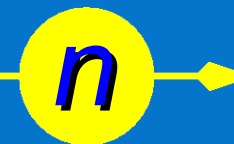
Polarisation support added



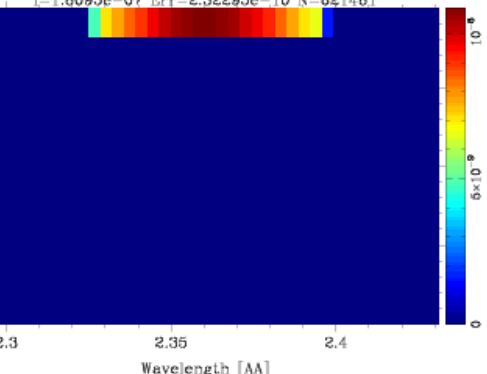
- First basic components added:
 - Spin flipper
 - Spin direction monitors
 - Vanadium with spin flip amplitudes
- More to come:
 - Peter Christiansen (Post Doc) recently hired for the purpose (Funding from ISIS TS2)
 - Hiring again in the near future, will announce at neutron@anl.gov



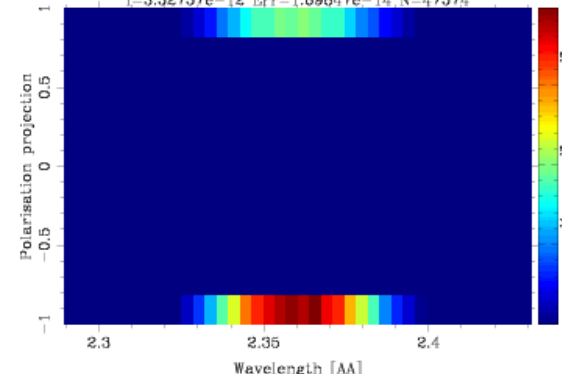
Polarisation support added



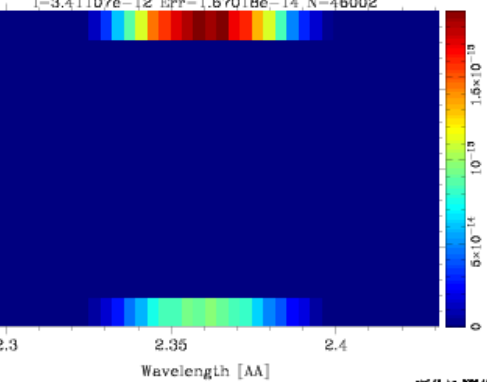
pollambdaMonitorFilter1 [pollambdaMonFilter1.data]
 X0=2.36097; dX=0.018909; Y0=0.909091; dY=1.84142e-08;
 I=1.8095e-07 Err=2.32295e-10 N=621481



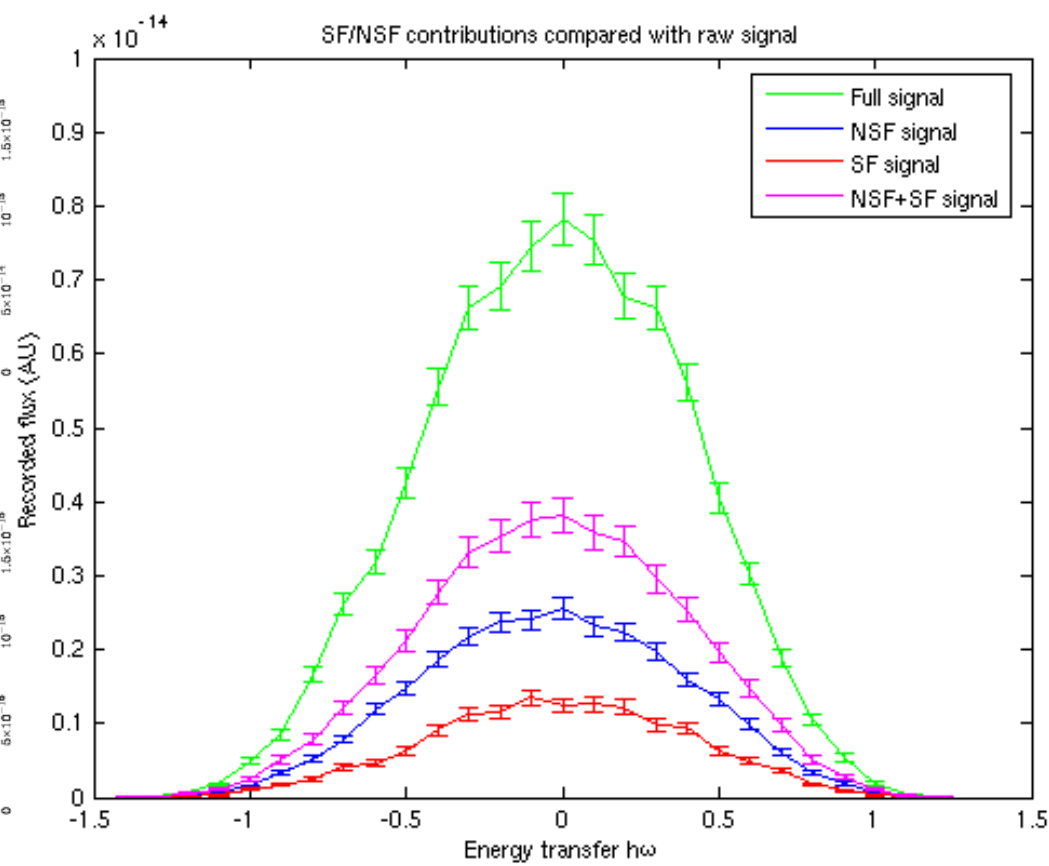
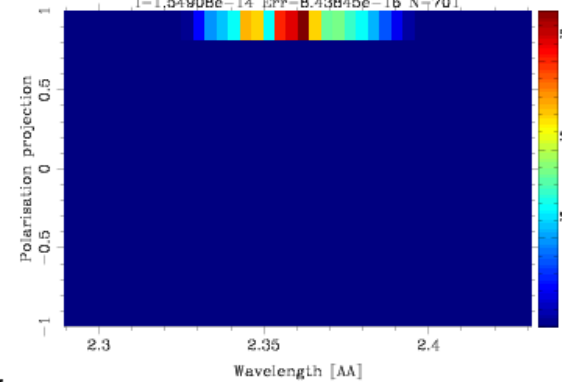
pollambdaMonitorSAMPLE [pollambdaMonSample.data]
 X0=2.36009; dX=0.0148277; Y0=-0.306615; dY=0.855823;
 I=3.52757e-12 Err=1.69847e-14 N=47574



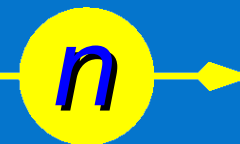
pollambdaMonitorMSF [pollambdaMonMSf.data]
 X0=2.36007; dX=0.0148289; Y0=0.305467; dY=0.856234;
 I=3.41107e-12 Err=1.67018e-14 N=46002



pollambdaMonitorFilter2 [pollambdaMonFilter2.data]
 X0=2.35933; dX=0.0143255; Y0=0.909091; dY=nan;
 I=1.54908e-14 Err=8.43845e-16 N=701



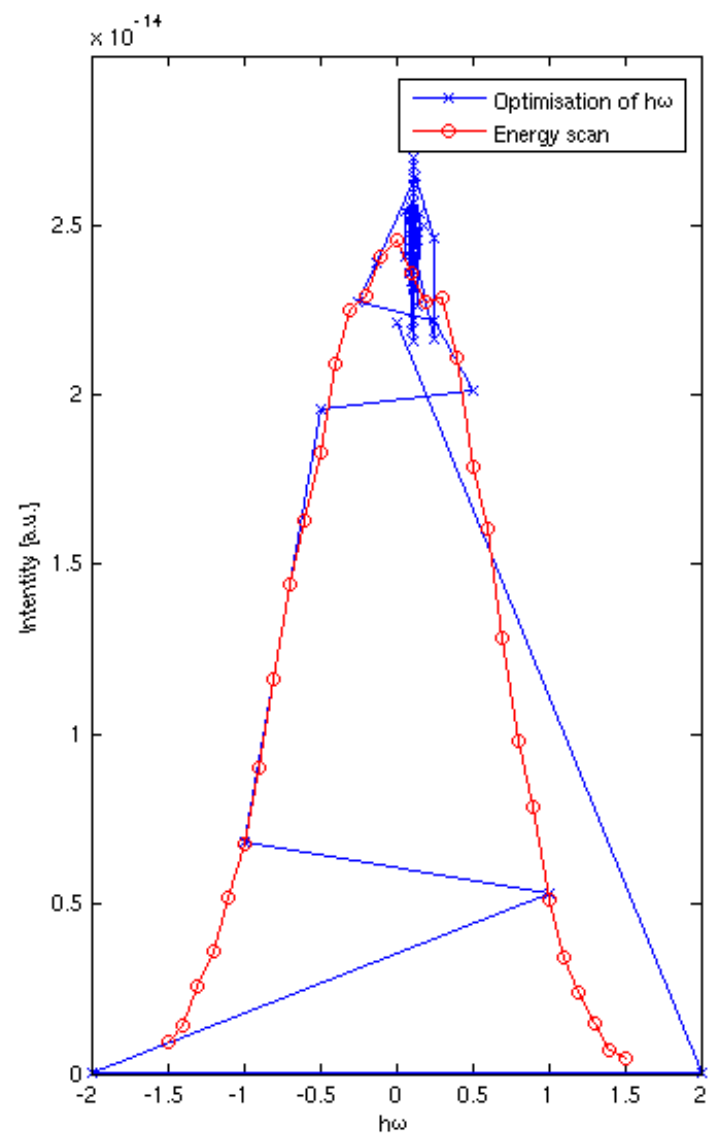
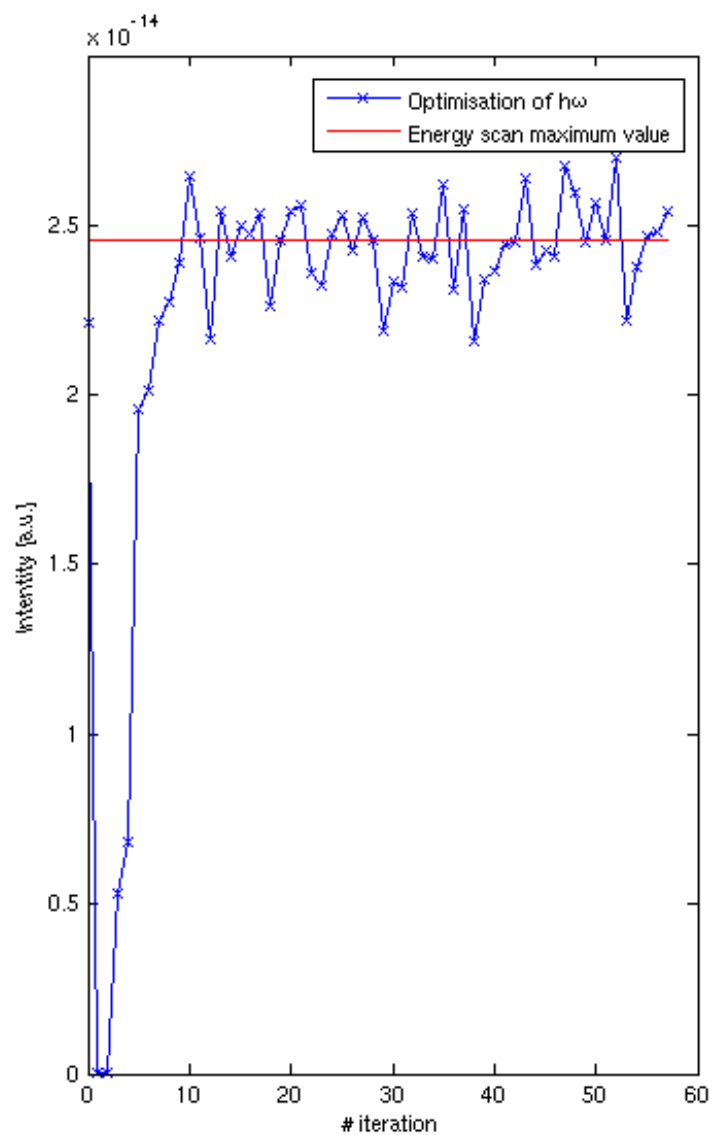
NEW TAS frontend template

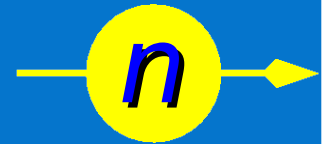


- Scan directly in reciprocal space, $\hbar\omega$ etc.
- Tested ILL Tasmad code
- Currently ILL IN20 (configurable), more will follow
- Easy resolution function calculation using Res_Sample



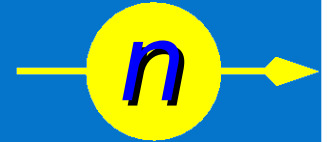
Optimisation support





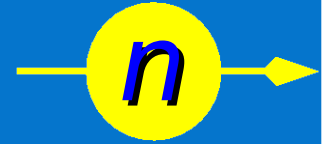
Release date

- 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

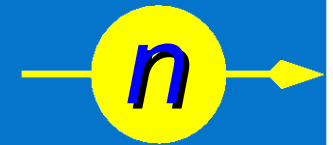
- Foresee increased work on components
- Emphasis on testing/validation using theory/data
- Virtual experiments
- Virtual neutron school
- Plan to seek funding for parallel effort in X-ray scattering (ESRF + Copenhagen Univ. interest)



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

 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'