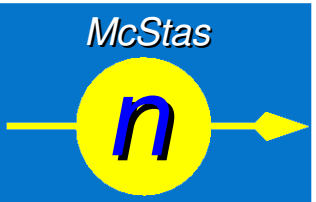


McStas 1.10

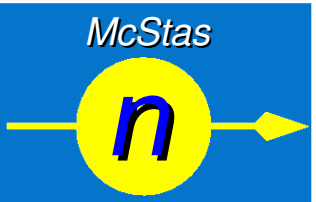
new release of the flexible neutron ray-tracing package - improved support for virtual experiments

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

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

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

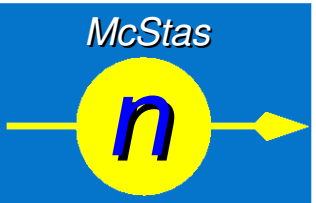
Agenda



- Very short intro
- New Features in 1.10
  - Language extensions, Polarisation support, Optimisation feature, reciprocal space calculator, TOF acceptance diagram on-the-fly
- Conclusion

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

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

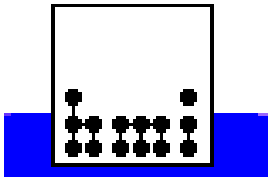
nmi3
EU Contract n°: HII3-CT-2003-505925

RISØ

McStas introduction

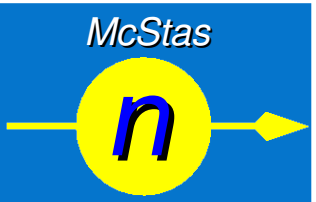
- Users at major labs





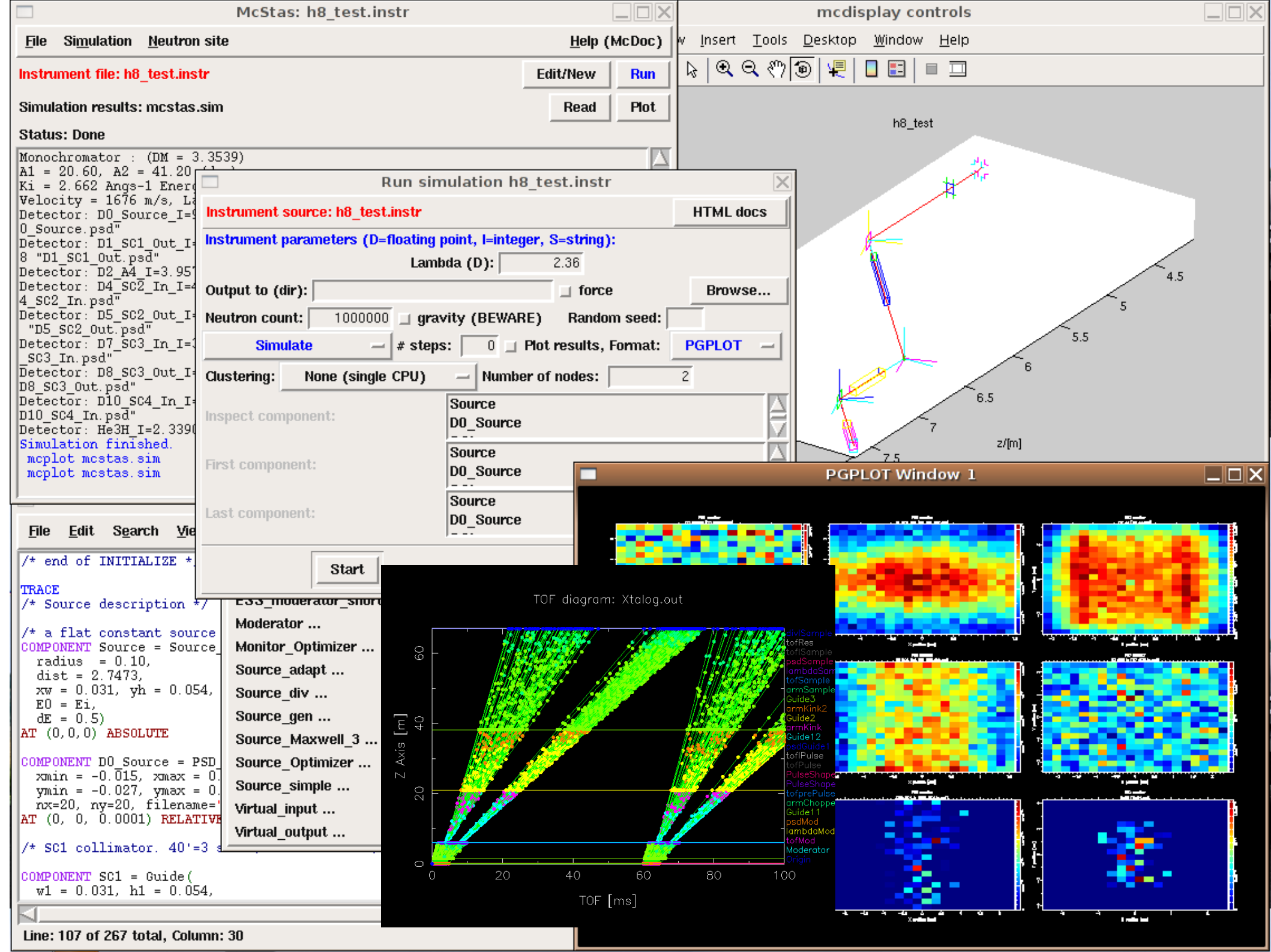

EU Contract n°: HII3-CT-2003-505925

McStas introduction

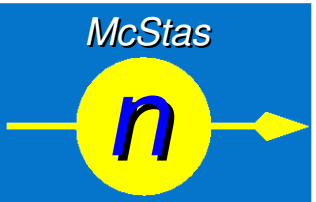


- Portable code (Unix/Linux/Mac/Win32)
- Write in (simple) 'instrument' language
- 'Component' files (~100) inserted from library
    - Sources, optics, samples, monitors
- If needed, write your own components
- GUI / commandline functionality
- Tools for plotting and datahandling included

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


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

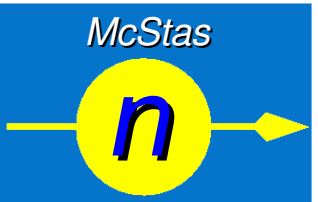
Implementation



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

EU Contract n°: HII3-CT-2003-505925

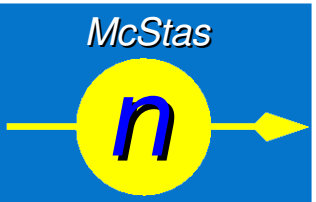
What is McStas used for?



- Instrumentation
  - Planning
  - Optimization
- Virtual experiments (See E Farhi talk)
- Data analysis
  - “I am seeing this strange effect, could it be due to....”
- Test spectrometer for students and novice users

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

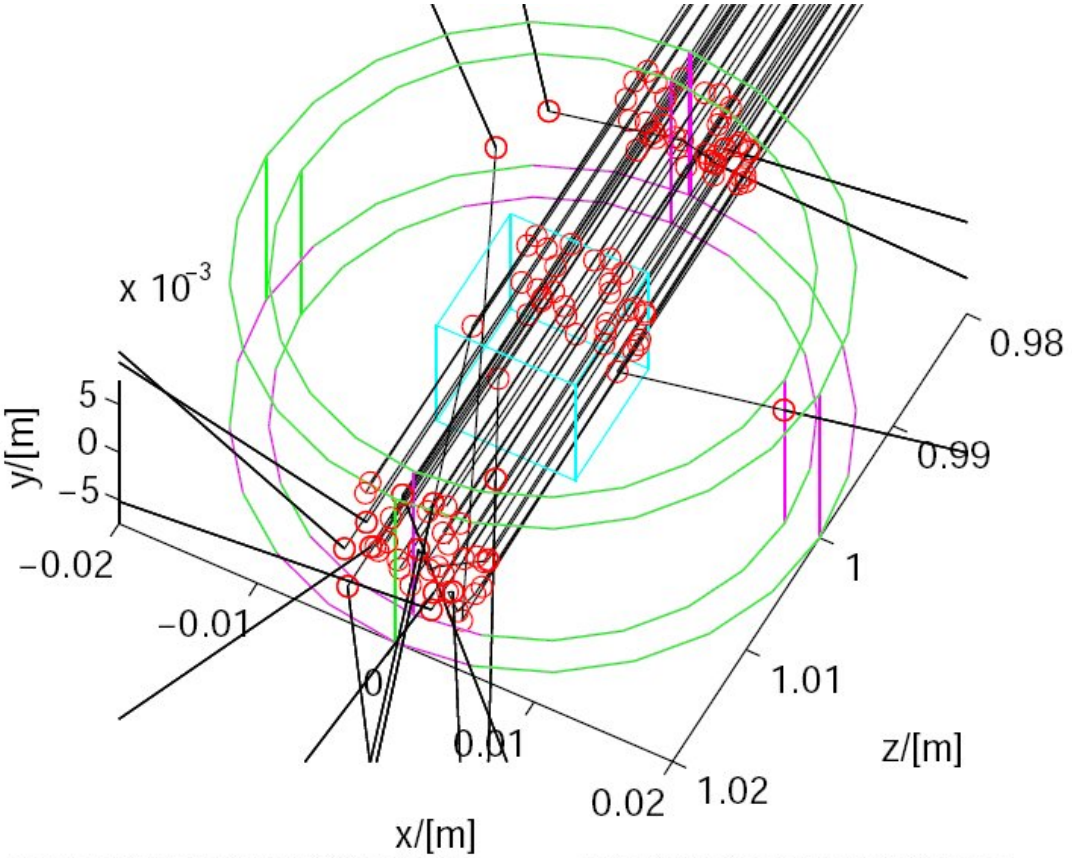
New Features



- Feature highlights from mcstas-1.10 (november 2006)

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

New – concentric comps

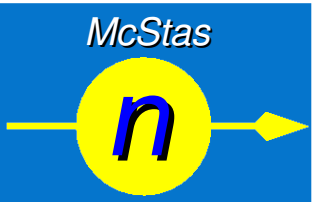


Components *inside* components.

Example: Liquid He (Isotropic_Sqw) inside Al Cryostat.

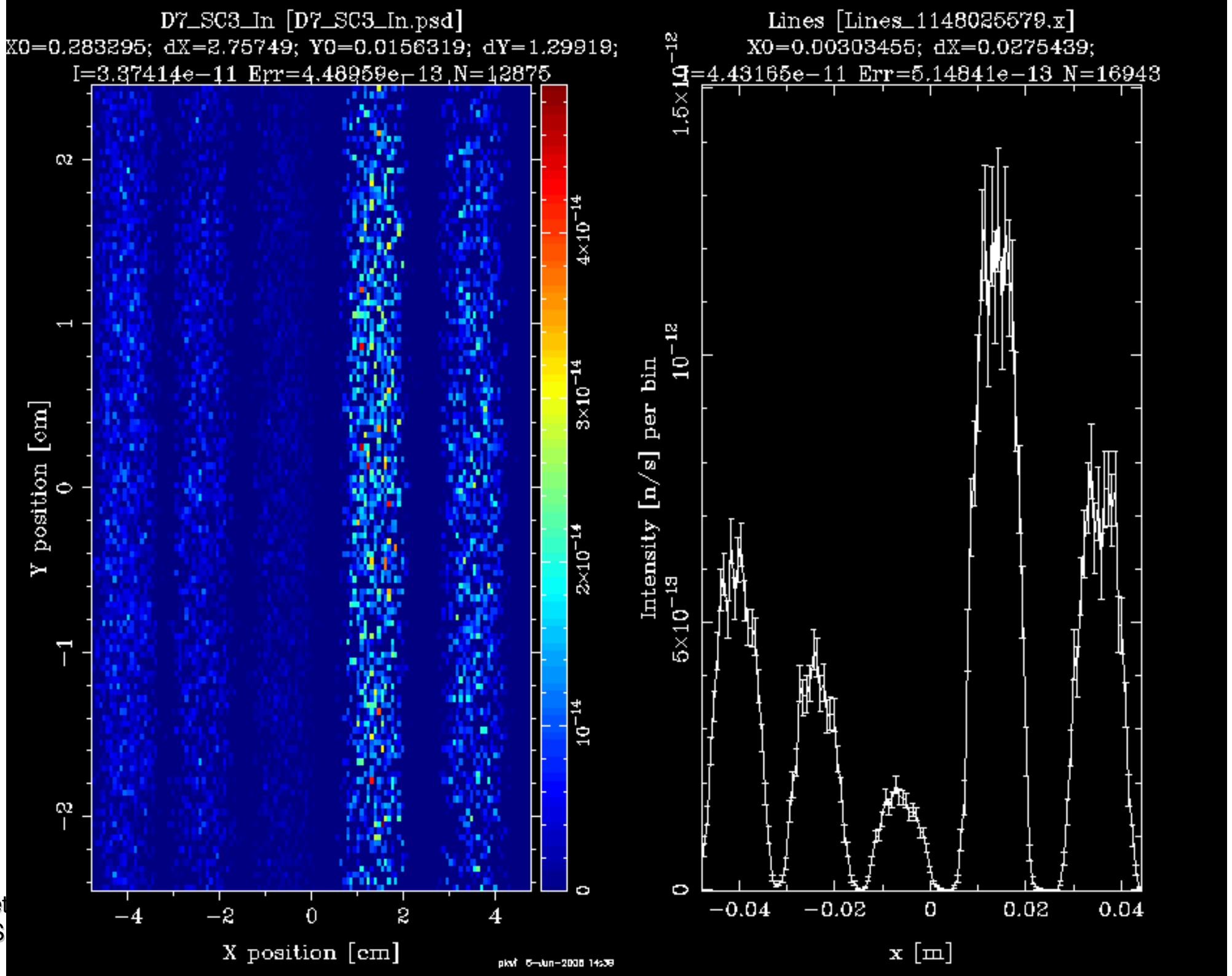
Al Powder lines separated from He rotons.

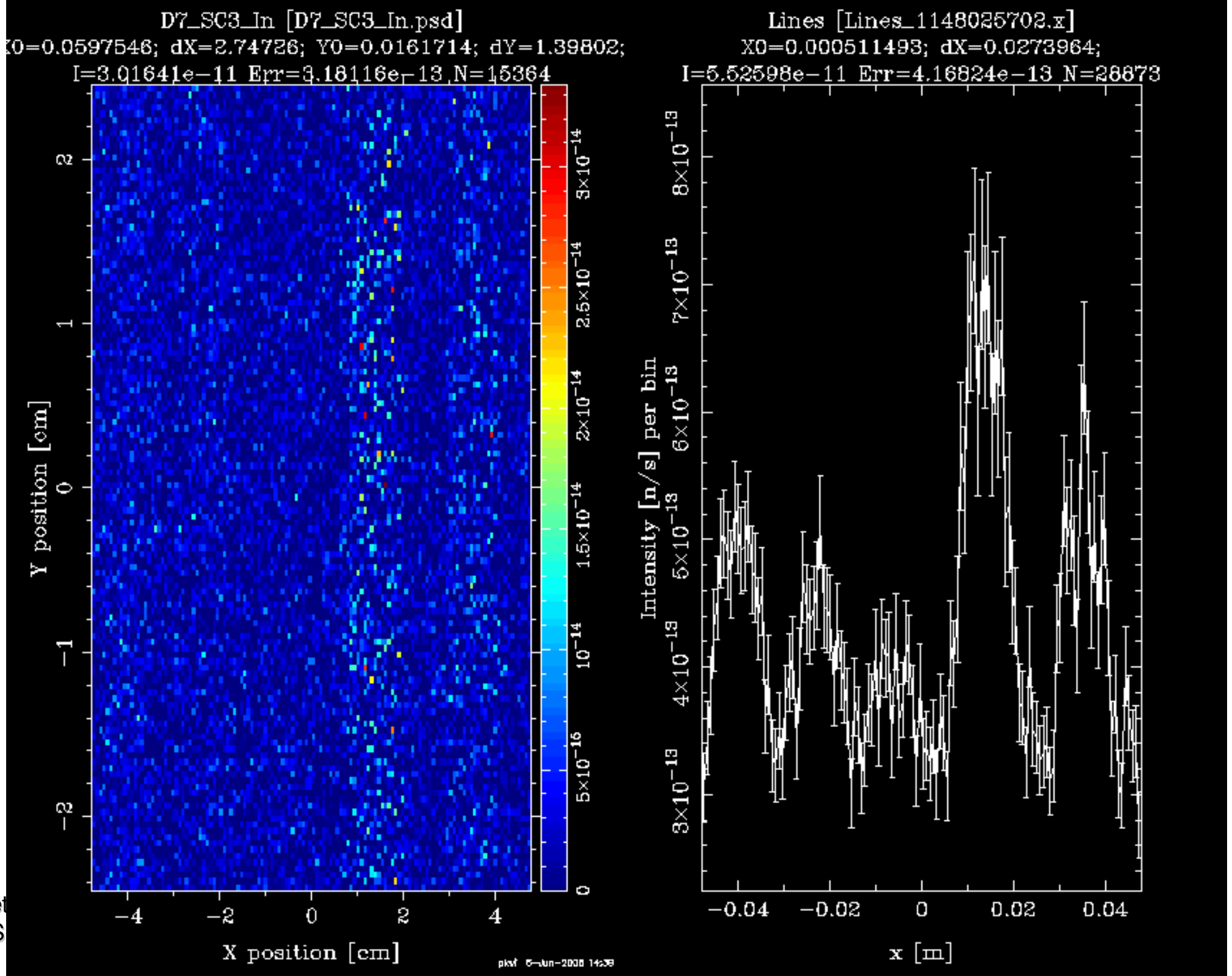
New – WHEN keyword

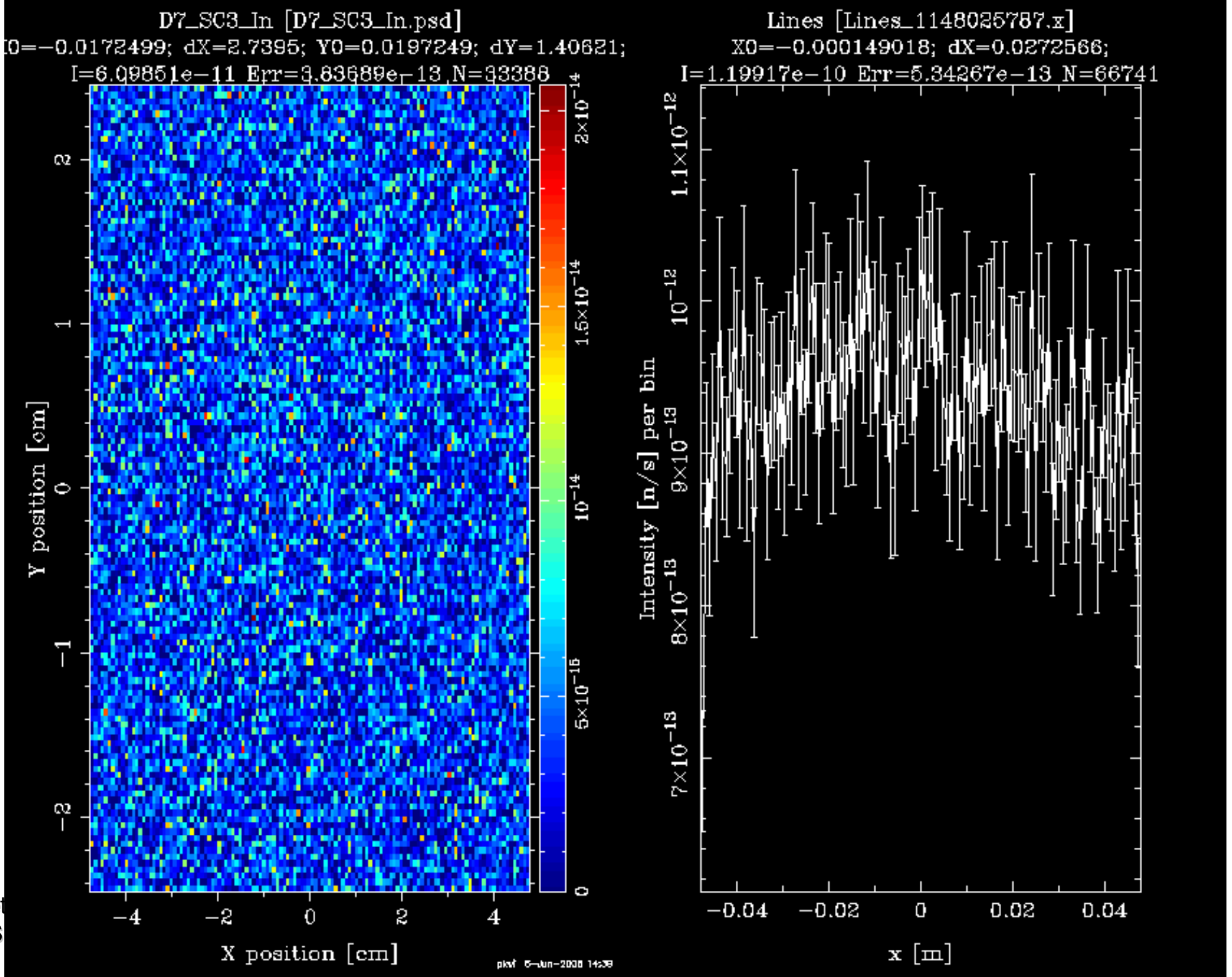


- *Mix* contributions from several scattering components
  - Phonon + Single crystal / ...
- Use to *parametrize* which sample component to use
  - Vanadium/Powder/Single crystal/...
- Use to *skip* certain parts of the instrument in certain configurations
  - With/without collimator

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


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
Y position [cm]
X position [cm]
Lines [Lines_1148025579.x]
X0=0.00303455; dX=0.0275439;
I=4.43165e-11 Err=5.14841e-13 N=16943
Intensity [n/s] per bin
x [m]


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
Y position [cm]
X position [cm]
Lines [Lines_1148025702.x]
X0=0.000511493; dX=0.0273964;
I=5.52598e-11 Err=4.16824e-13 N=28873
Intensity [n/s] per bin
x [m]

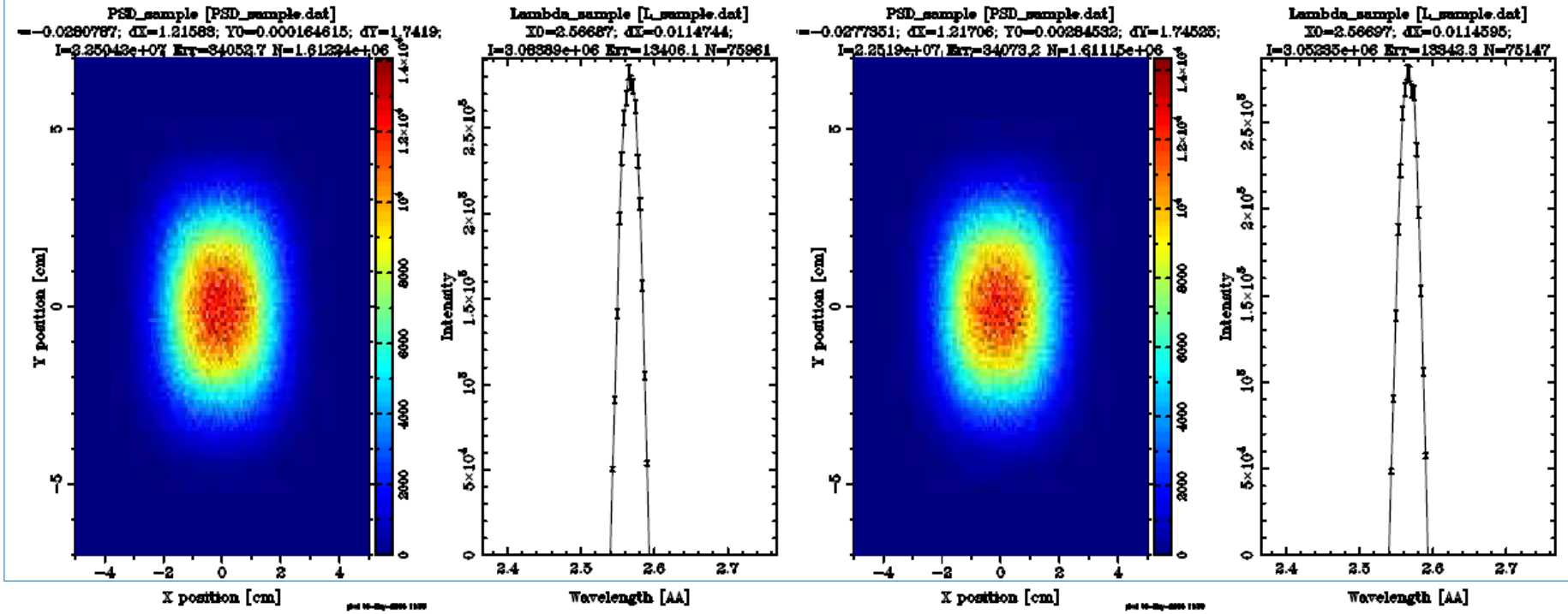

D7_SC3_In [D7_SC3_In.psd]
X0=-0.0172499; dX=2.7395; Y0=0.0197249; dY=1.40621;
I=6.09851e-11 Err=3.83689e-13 N=33388
Y position [cm]
X position [cm]
pkf 6-Jun-2008 14:38
Lines [Lines_1148025787.x]
X0=-0.000149018; dX=0.0272566;
I=1.19917e-10 Err=5.34267e-13 N=66741
Intensity [n/s] per bin
x [m]

New – JUMP keyword

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

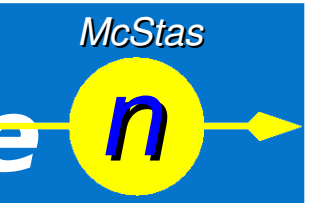
Example: 49 versus 1 guide element for curved guide desc.

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



nmi3 EU Contract n°: RII3-CT-2003-505925

NEW TAS frontend template



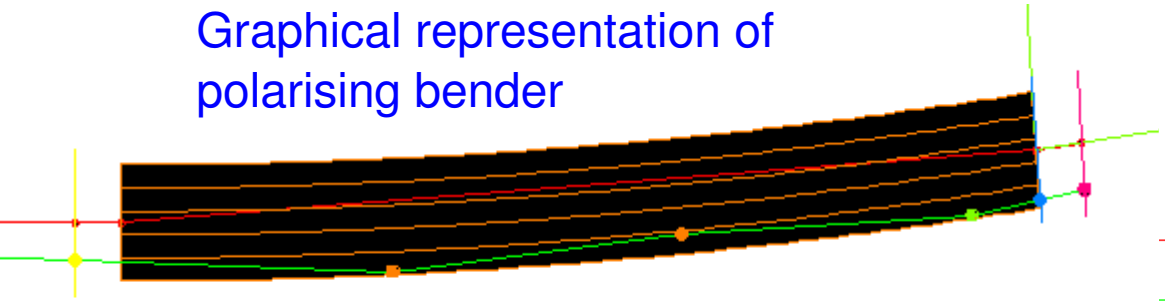
- Scan directly in reciprocal space, $\hbar\omega$ etc.
- Tested ILL Tasmad code
- Currently ILL IN20 (configurable), more will follow
- Easy resolution function calculation using Res_Sample
- Cooper-Nathans method still needs to be implemented

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

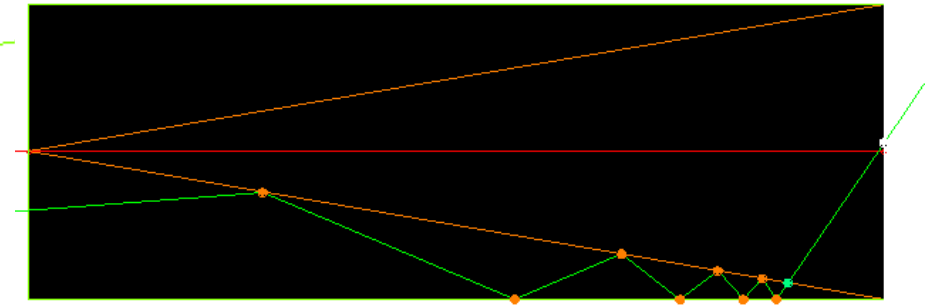
Polarisation in McStas

- Support under development (started spring 2006, will be in mcstas-1.10)
- Work primarily by Peter Christiansen (RISØ), input from Rob Dalgliesh (ISIS)
- Full 3D polarisation handling
- Main components:
  - Monochromator_pol.comp (Polarising monochromator/analyzer)
  - Pol_bender.comp (Polarising bender)
  - Pol_guide_vmirror.comp (Guide with semi-transparent, polarising mirror)
  - Pol_mirror.comp (Polarising mirror)
  - Pol_simpleBfield.comp (Numerical precession in analytical magnetic fields)
  - Polarisation monitors

Graphical representation of polarising bender



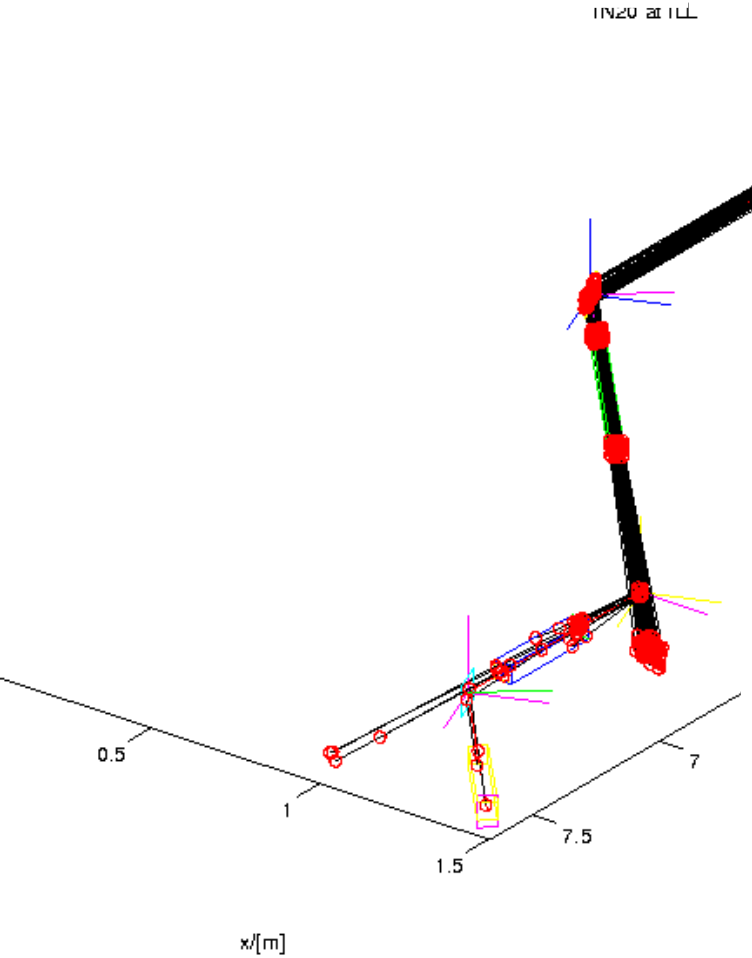
Graphical representation of guide with polarising vmirror

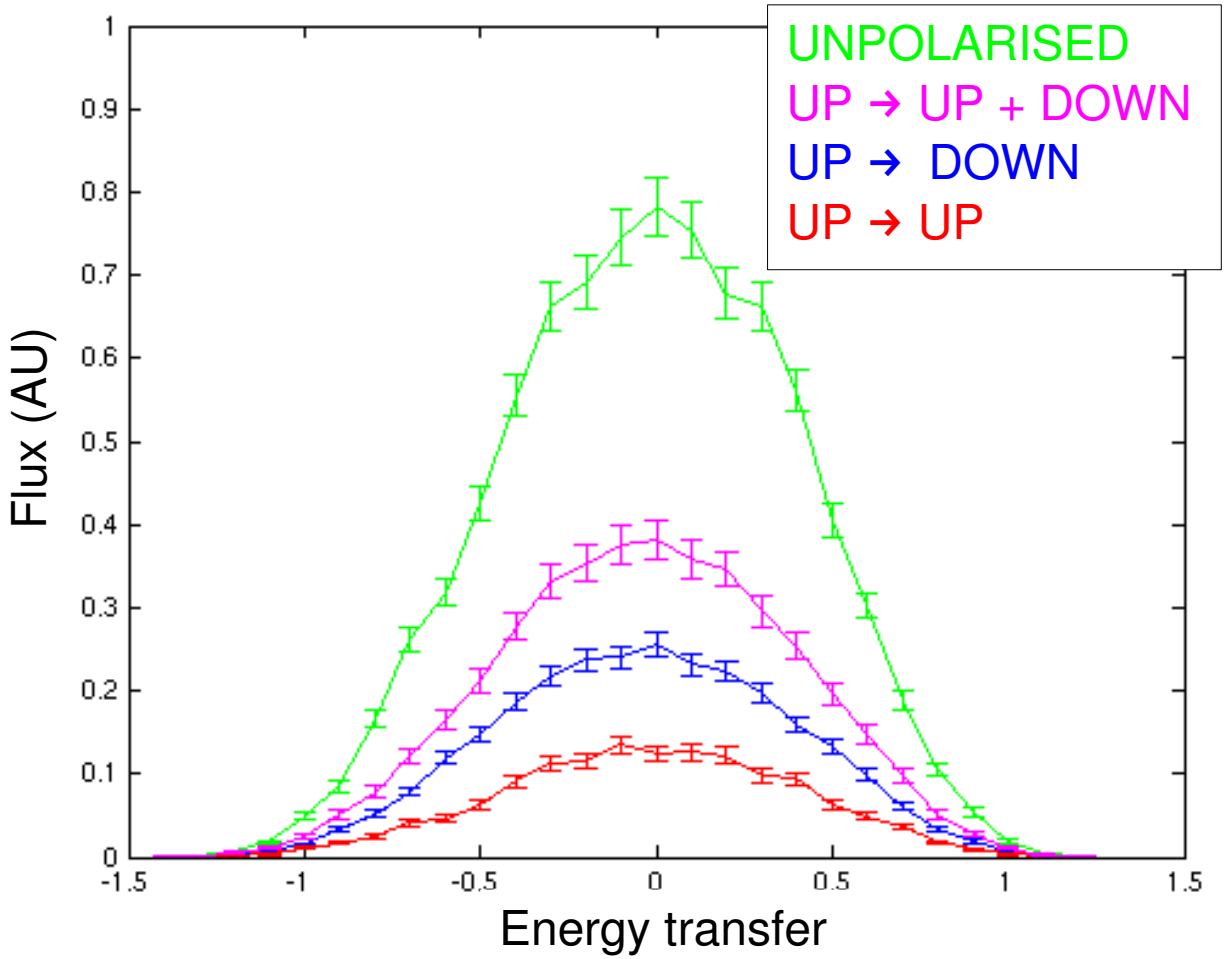


NOTE: Peter Christiansen has left McStas, for continuation RISØ is hiring a 2 year Post Doc

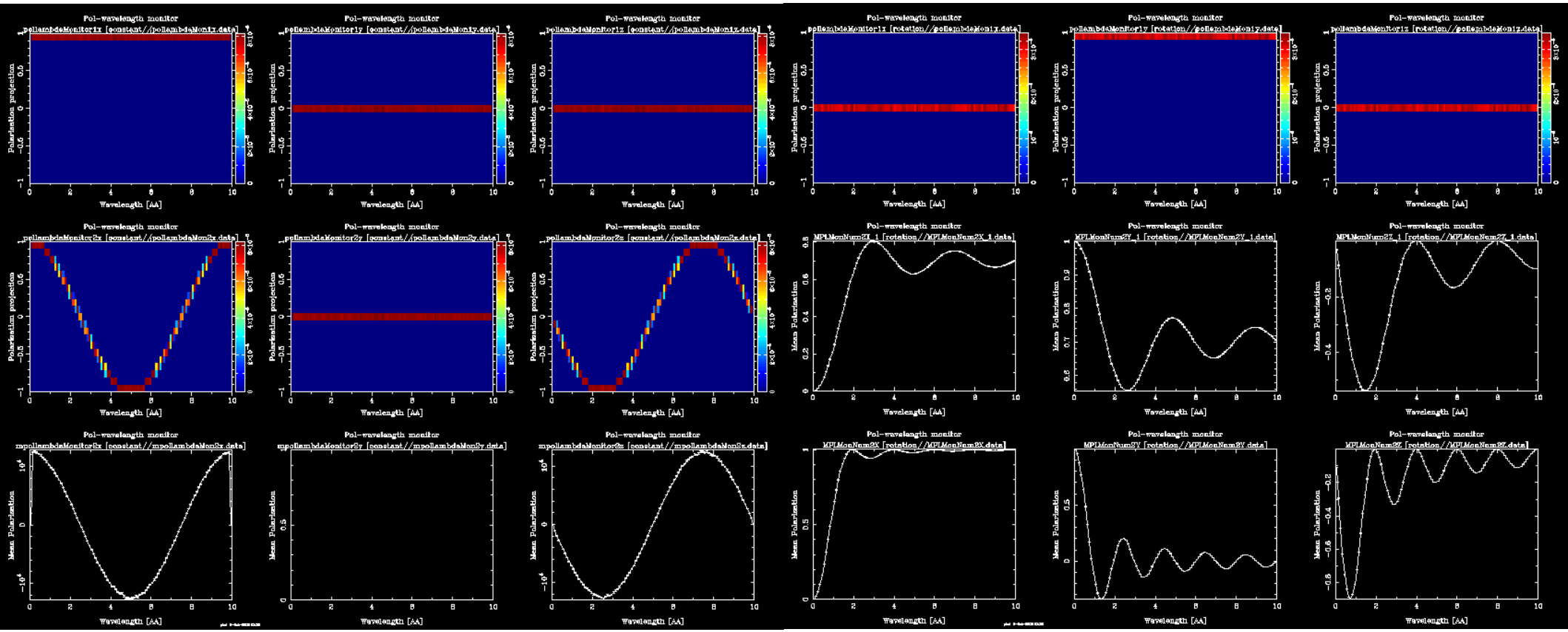
EU Contract n°: HII3-CT-2003-505925

TAS + Vanadium, NSF+SF



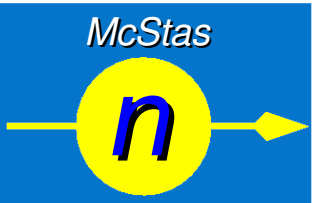


McStas: Reproducing graphs from the litterature (Seeger & Daemen)



EU Contract n°: HII3-CT-2003-505925

Tool/Core workover



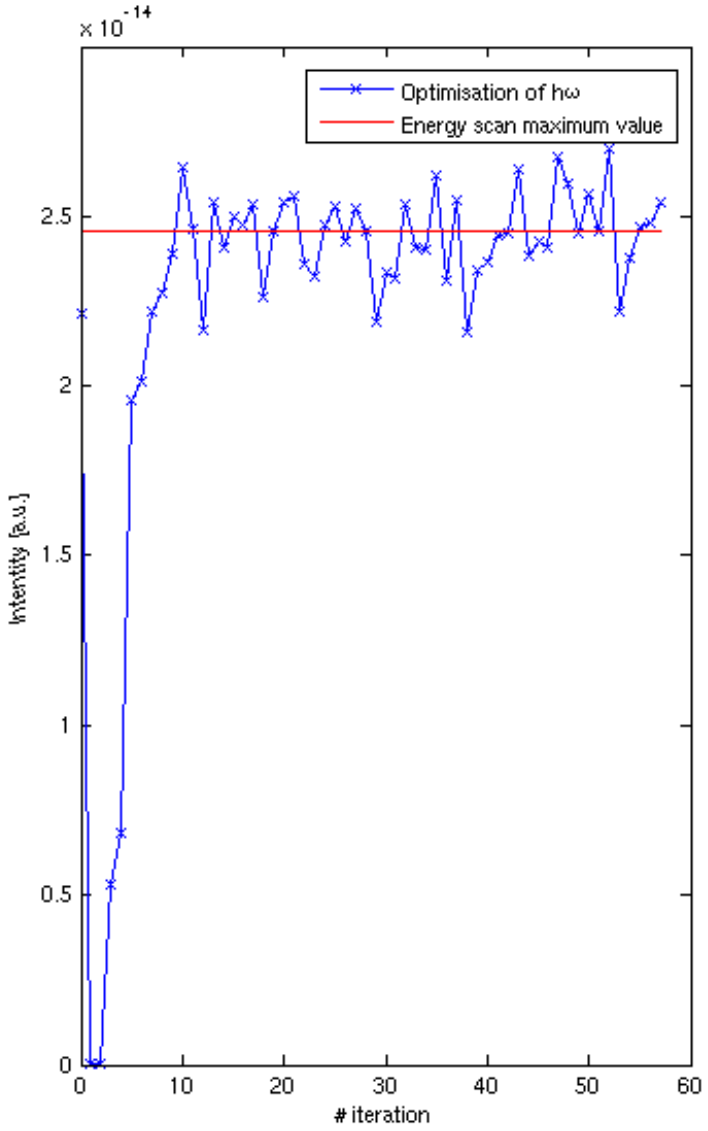
General package workover

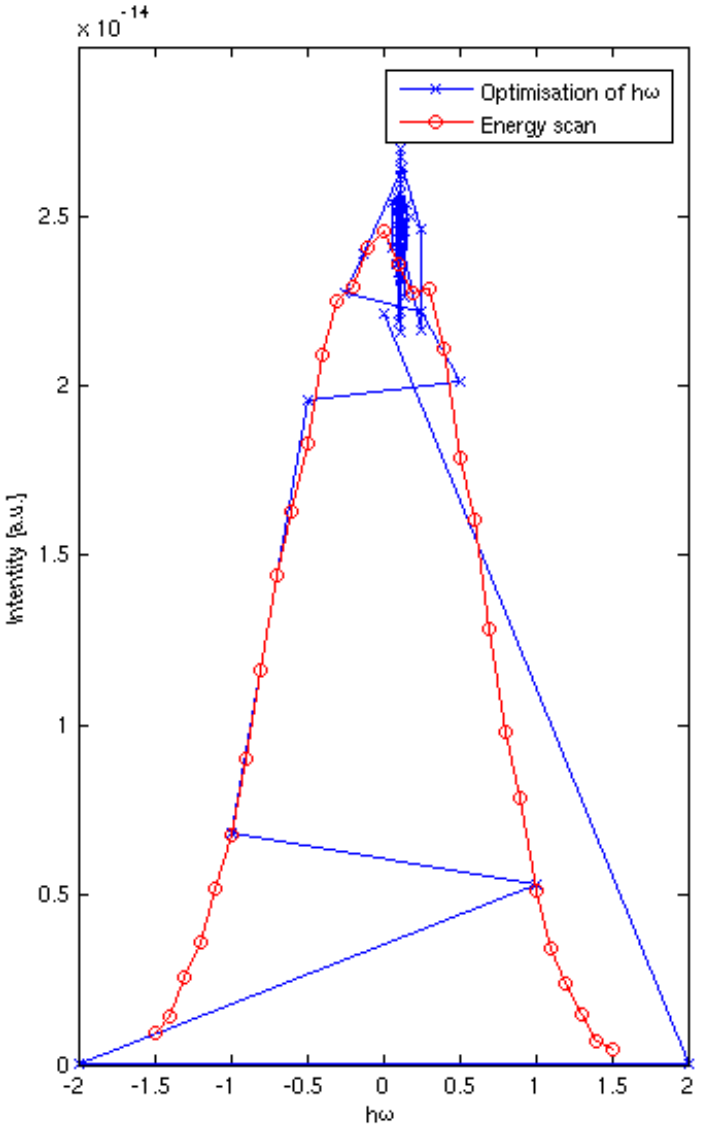
- Support for read-in of MCNP event files
- New 'merging/conversion' tool mcformat (Can assemble a scan dataset from similar subfolders – GRID use)
- The new McStas release supports POSIX threading on multi-core processors. Same mechanism used when running on Grids/clusters (MPI recommended).

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

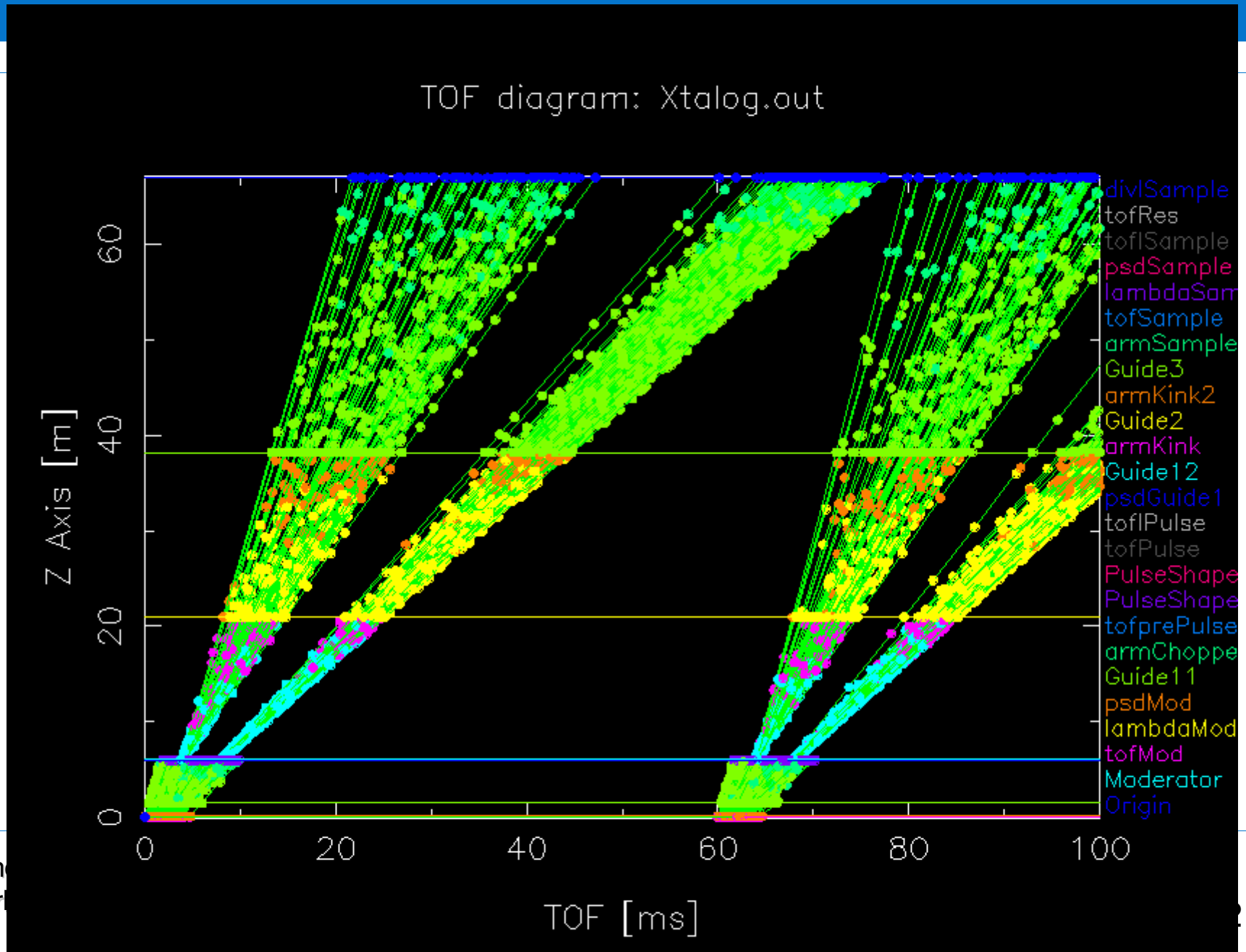
Optimisation support

McStas

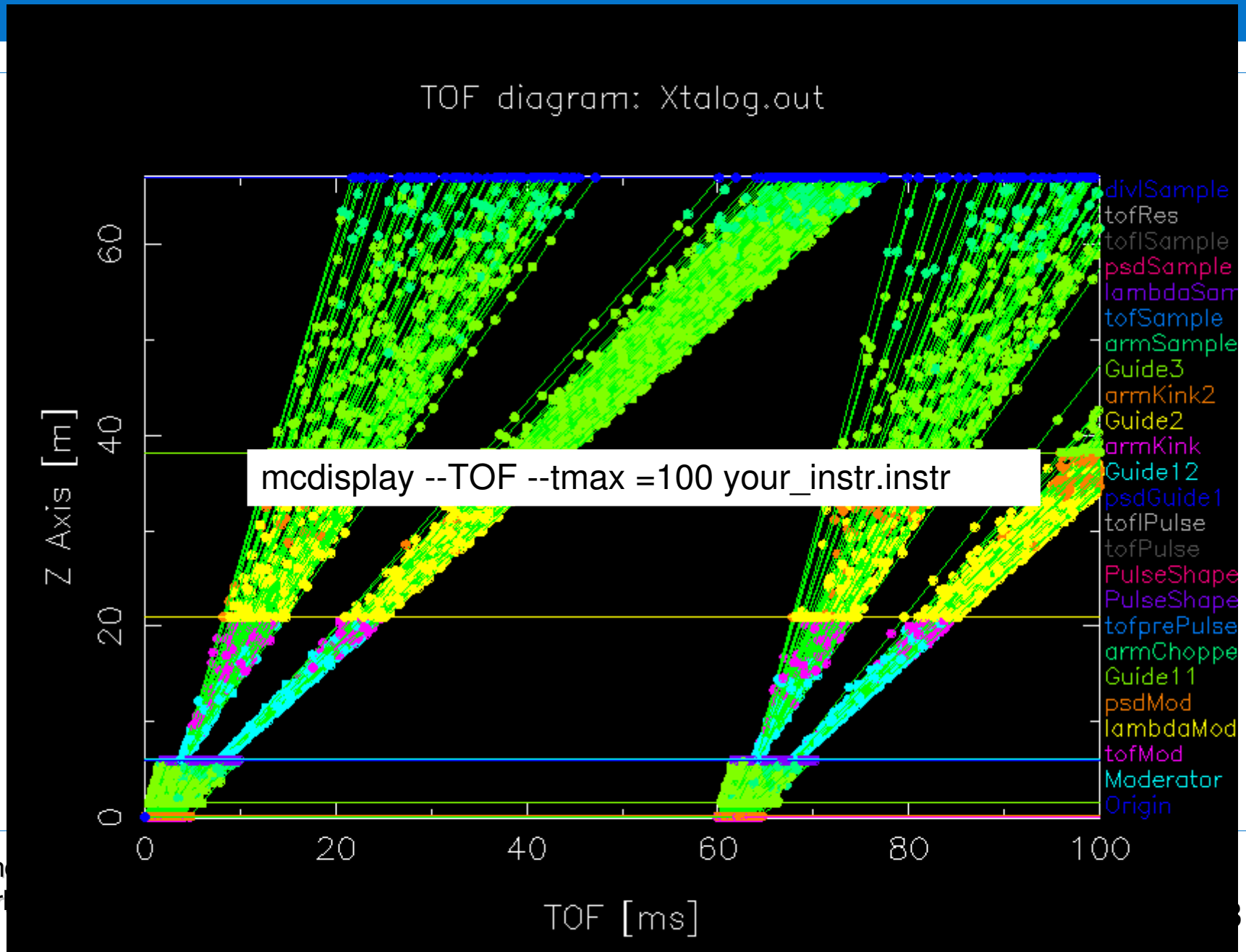




TOF acceptance diagrams



TOF acceptance diagrams

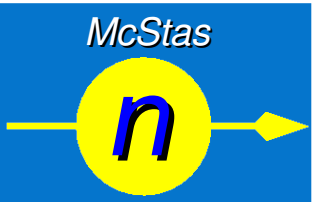


Release date

- Planned release date of McStas 1.10 in November 2006
- Subscribe to neutron-mc@risoe.dk to stay informed (see http://www.mcstas.org)

EU Contract n°: HII3-CT-2003-505925

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)

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

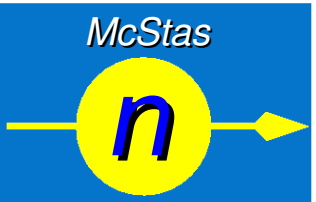
Funding

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

  EU Contract n°: HII3-CT-2003-505925

- Hope to be in FP7 as well.
- Contributions (manpower, code, 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
  - TOF Chopper acceptance diagrams
  - Focus now on:
  - Testing / validation of existing components
  - Virtual experiments
- Future:
  - Possibly X-ray 'sister-package'

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