McStas
a Monte Carlo ray-tracing package for neutrons

24 February 2009, ESRF

Kim Lefmann,

Niels Bohr Institute, Univ. Copenhagen

Peter Willendrup

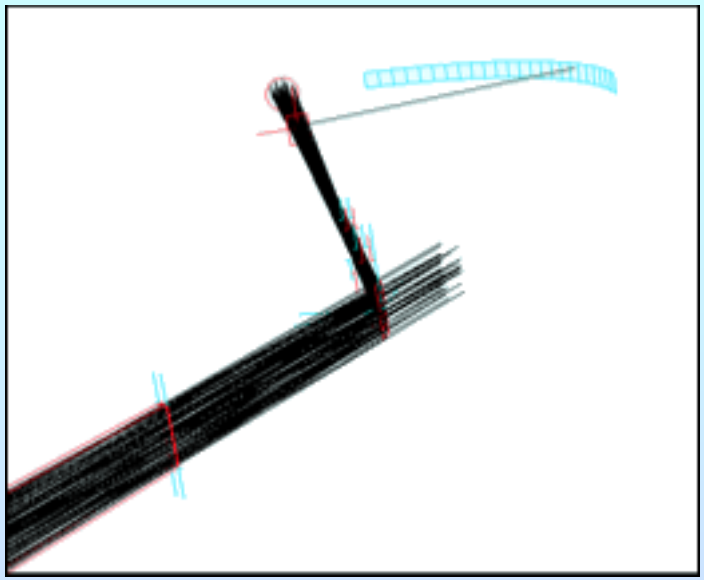
RISØ DTU

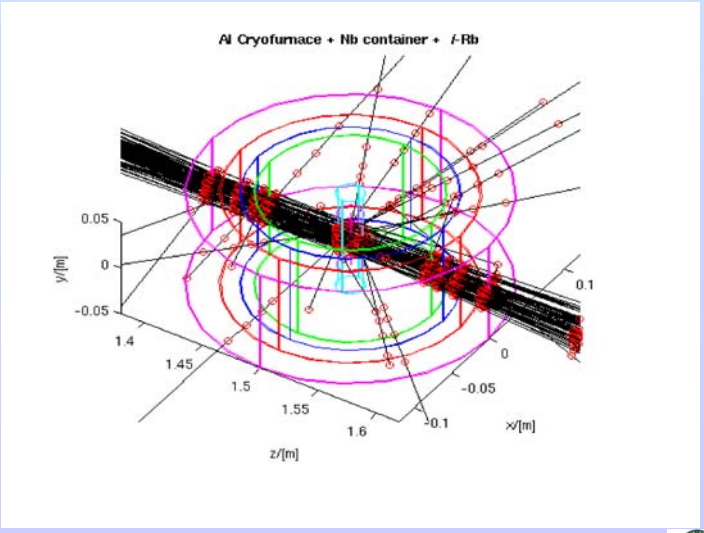
Outline

- The McStas package
- Validation of results
- Virtual experiments for science and education
- The future of McStas

McStas in brief

- Ray-tracing:
  - Follow rays through the entire instrument
  - Neutrons: 10 co-ordinates (**r**,**v**,**s**,t)
  - … and the weight, p
- Monte-Carlo:
  - Random selection of start parameters
  - … and others if needed
- The McStas package:
  - Risø / ILL / Copenhagen
  - Handles geometry
  - Library of tested components
  - User interface
  - Open source:
  - Many contrib. from community

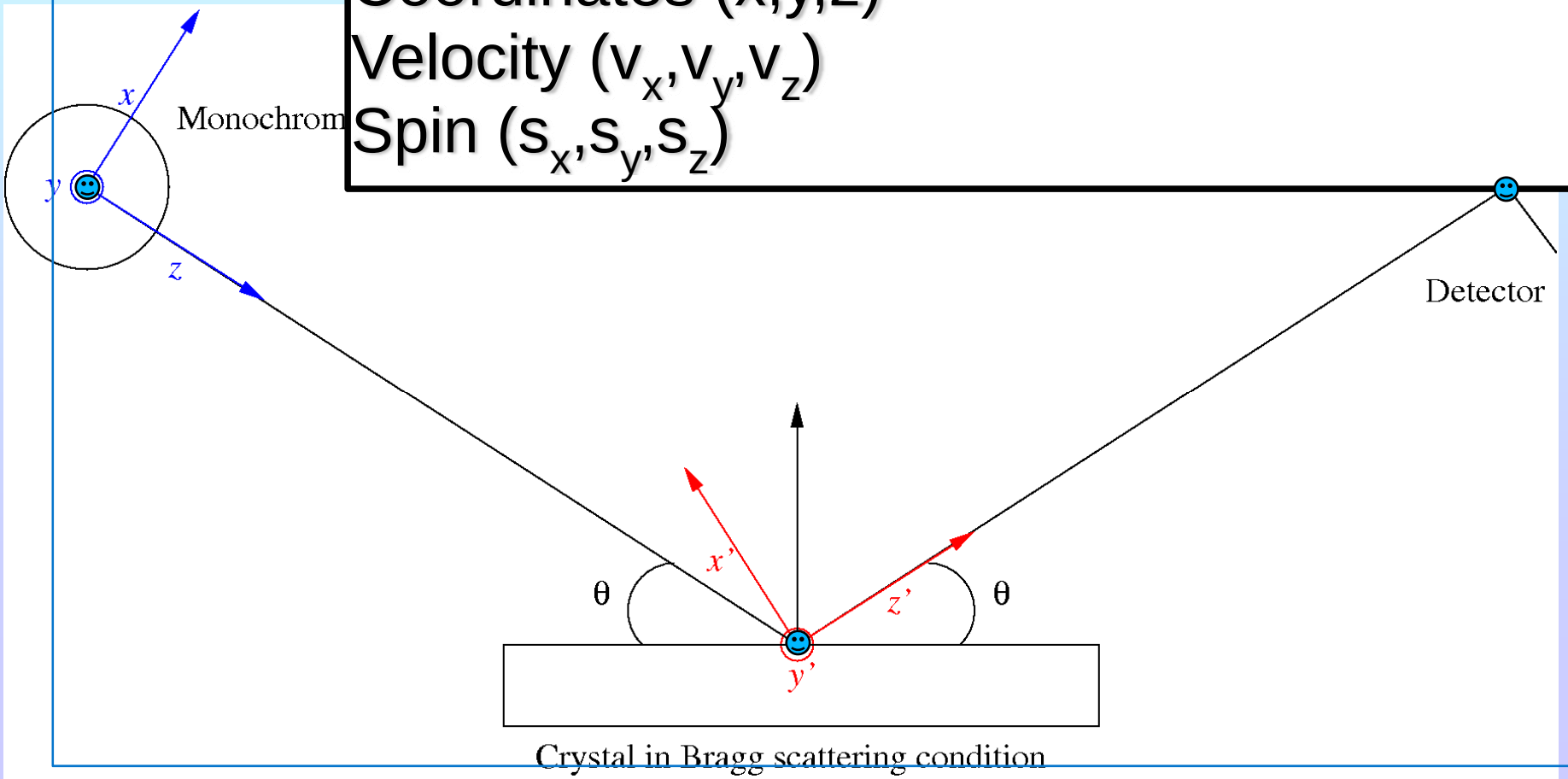




McStas neutron rays

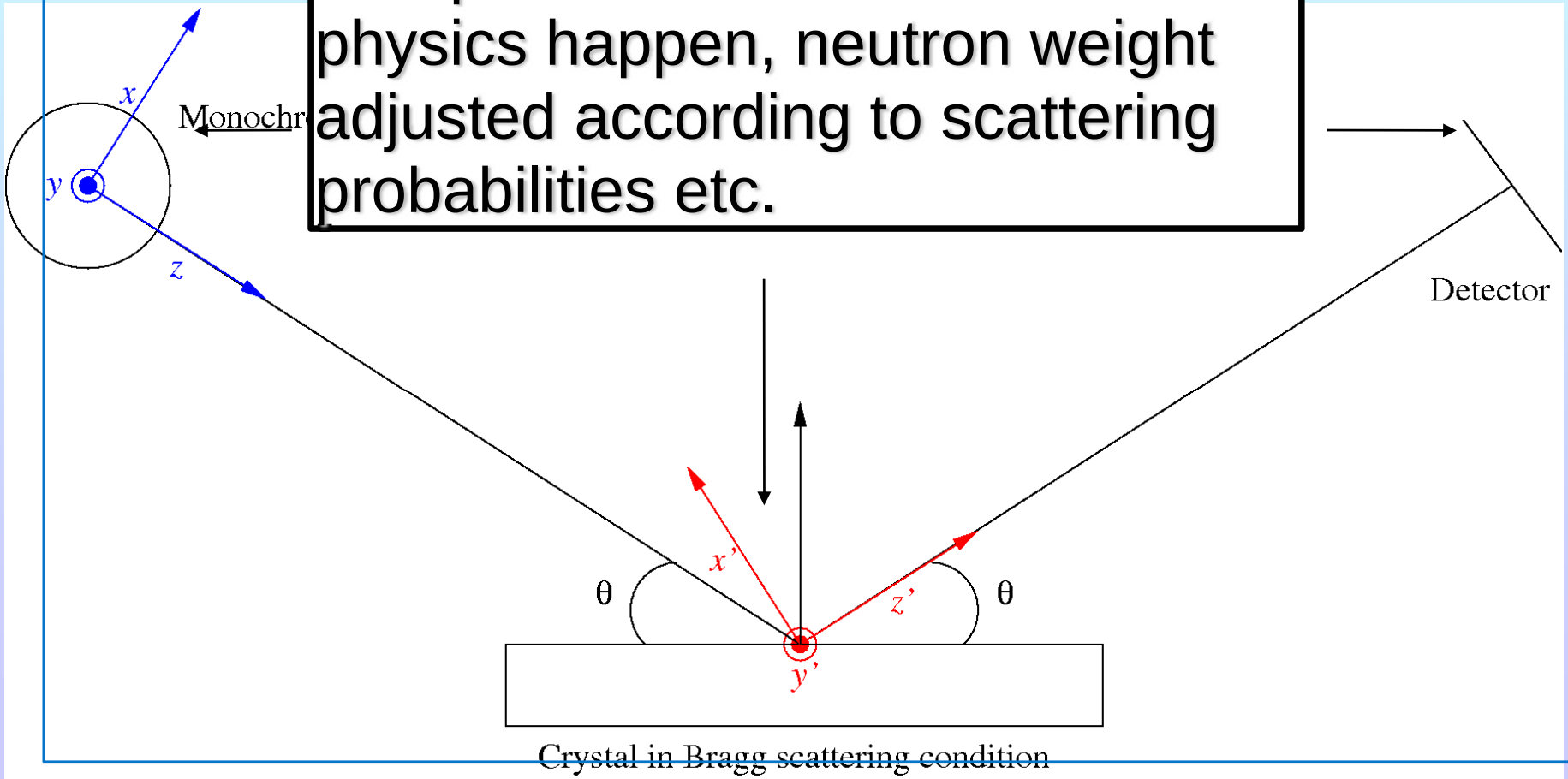
Neutron ray/package:

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)



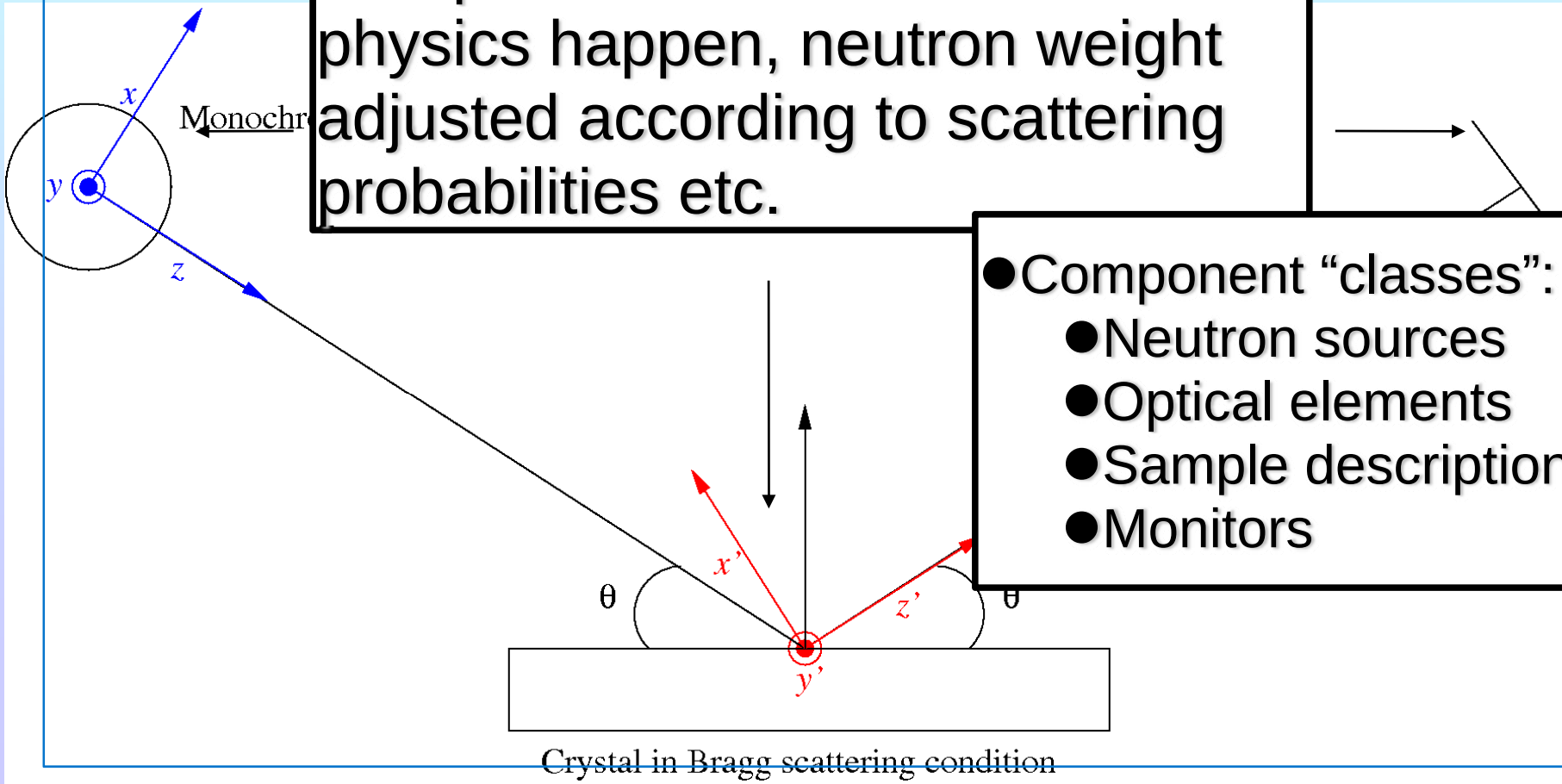
McStas components

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



McStas components

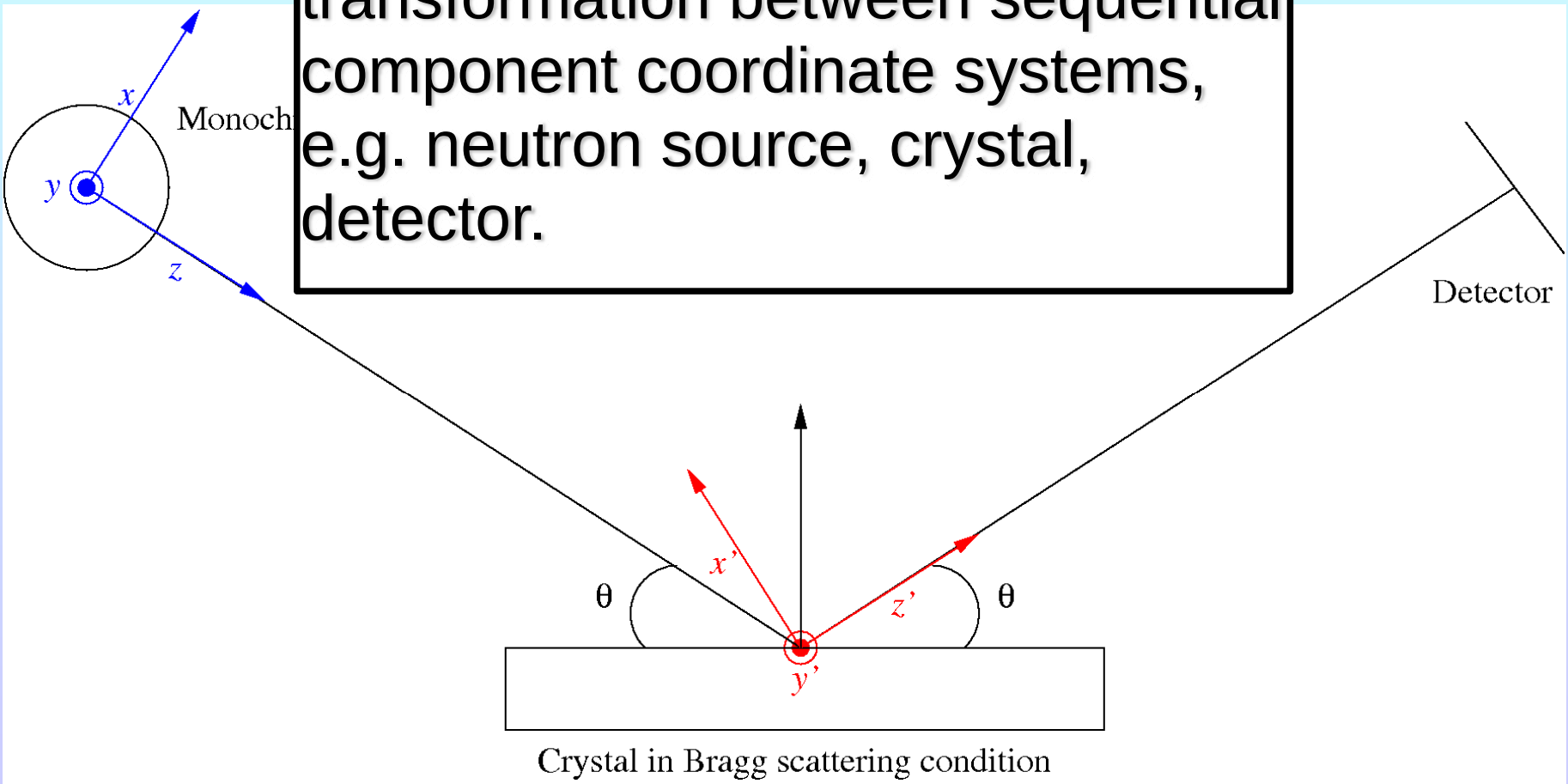
Components: Here the neutron physics happen, neutron weight adjusted according to scattering probabilities etc.



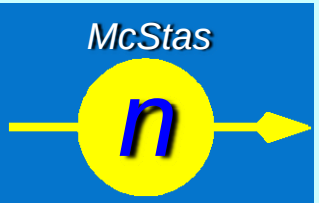
- Component “classes”:
  - Neutron sources
  - Optical elements
  - Sample descriptions
  - Monitors

McStas instrument

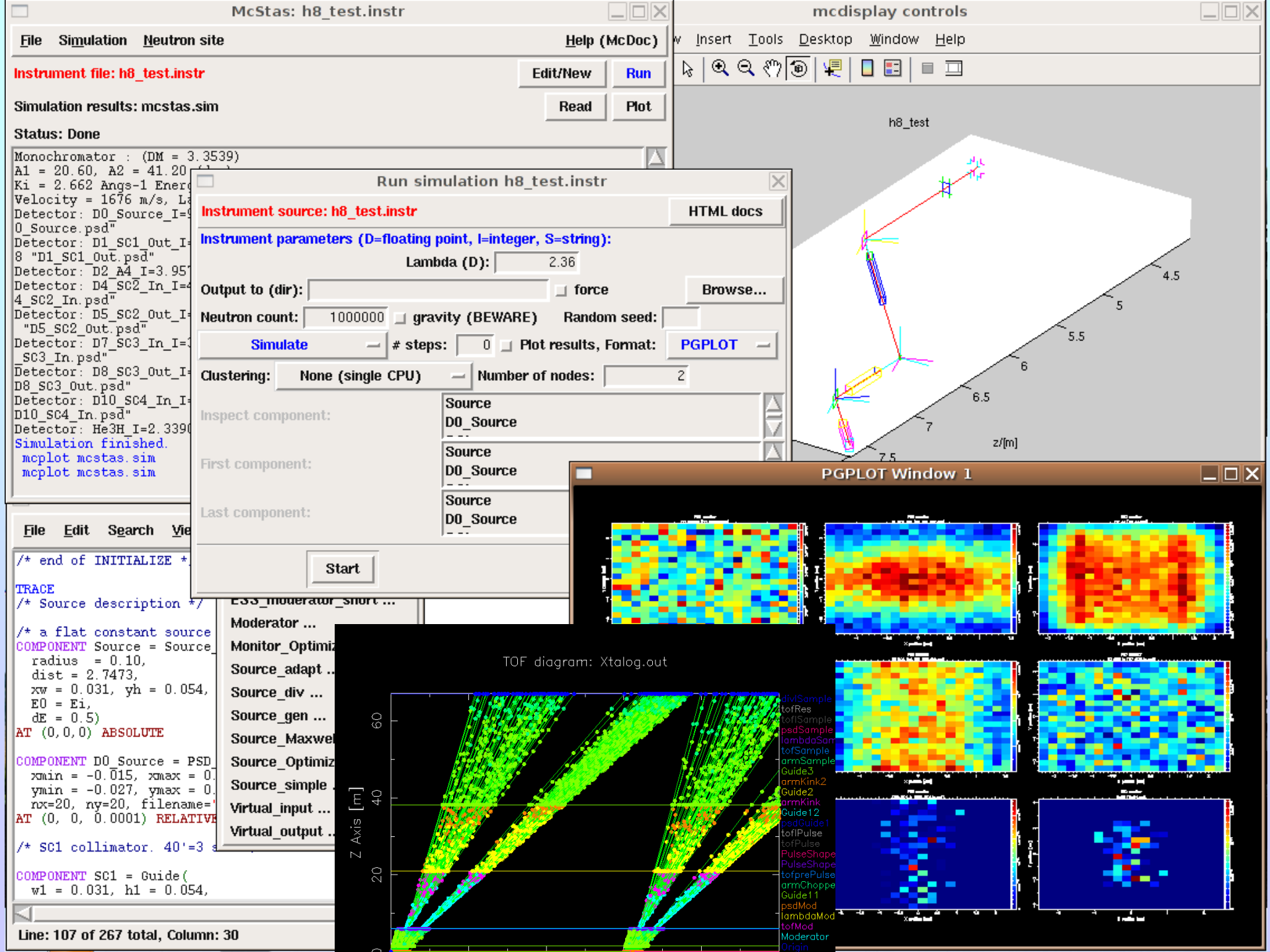
Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.



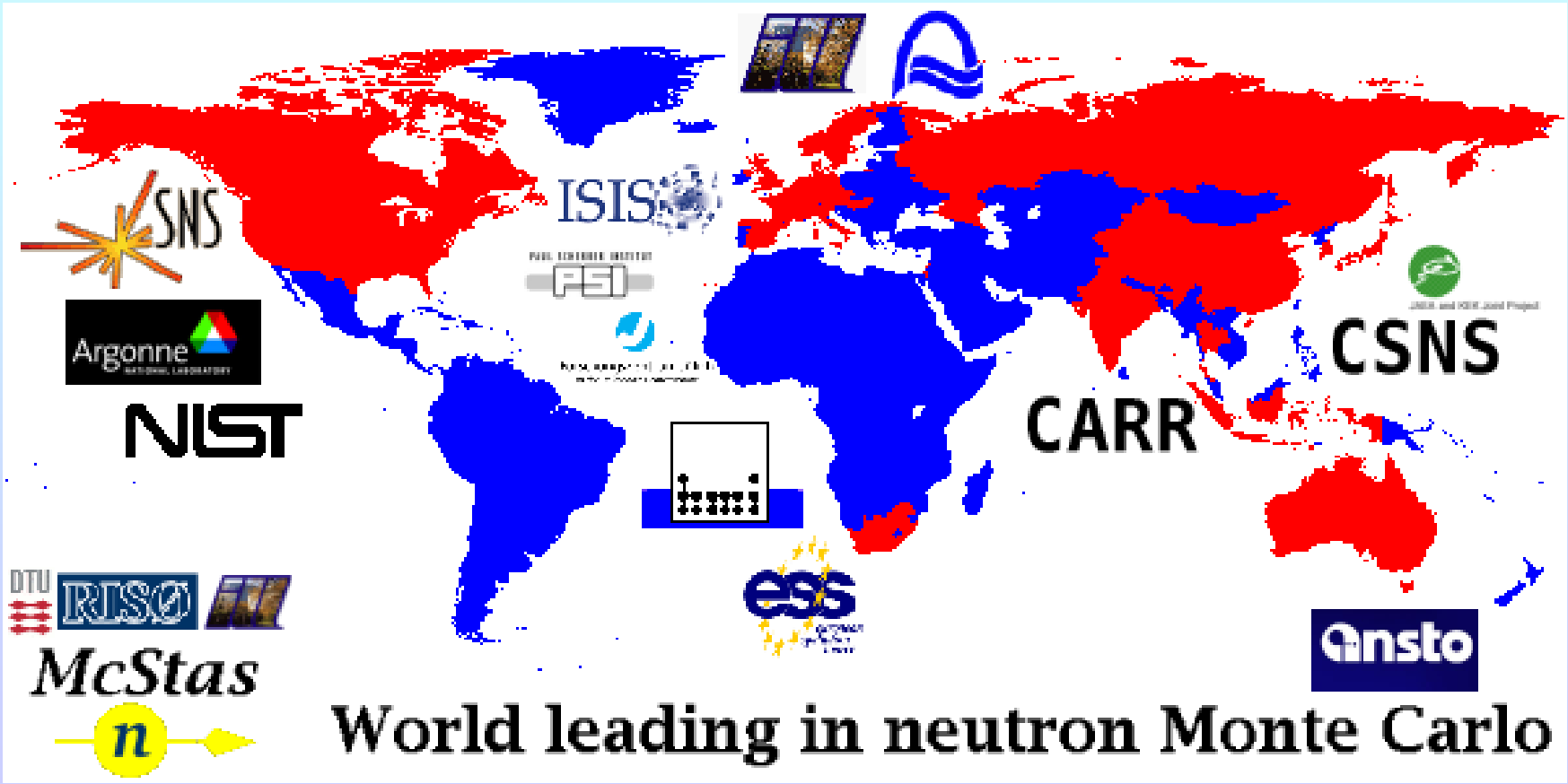
McStas overview



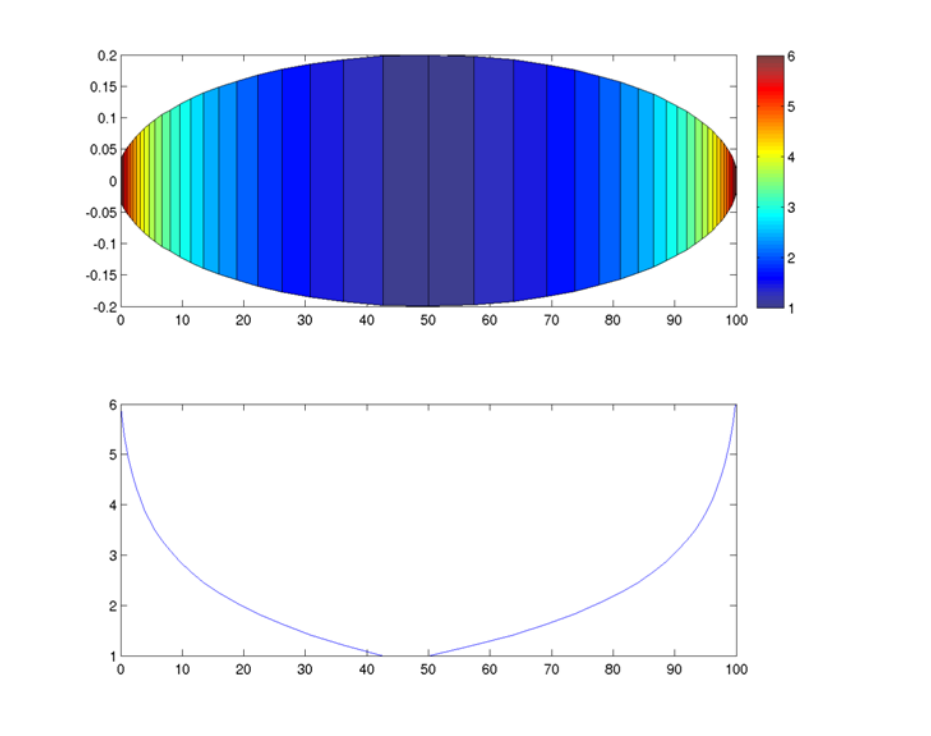
- Portable code (Unix/Linux/Mac/Win32)
- Write in (simple) 'instrument' language
- 'Component' files (~100) inserted from library
  - Sources, optics, samples, monitors
- If needed, write your own components
- GUI / commandline functionality
- Tools for plotting and datahandling included

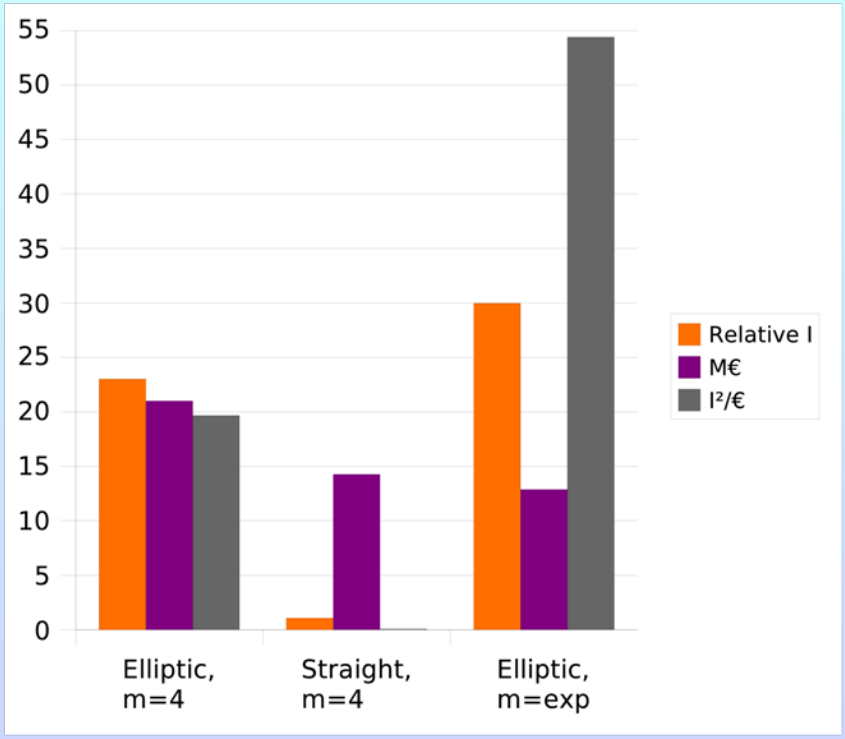

McStas: h8_test.instr
File Simulation Neutron site Help (McDoc)
Instrument file: h8_test.instr
Edit/New
Run
Simulation results: mcstas.sim
Read
Plot
Status: Done
Monochromator : (DM = 3.3539)
A1 = 20.60, A2 = 41.20
Ki = 2.662 Angs-1 Energ
Velocity = 1676 m/s, La
Detector: D0_Source_I=9
0_Source.psd"
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=1
_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
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
mcdisplay controls
w Insert Tools Desktop Window Help
h8_test
4.5
5
5.5
6
6.5
7
7.5
z/[m]
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
COMPONENT SC1 = Guide(
w1 = 0.031, h1 = 0.054,
Line: 107 of 267 total, Column: 30
Moderator ...
Monitor_Optimiz
Source_adapt ..
Source_div ...
Source_gen ...
Source_Maxwe
Source_Optimiz
Source_simple
Virtual_input ...
Virtual_output ..
PGPLOT Window 1
TOF diagram: Xtalog.out
Z Axis [m]
60
40
20
divSample
tofRes
tofISample
psdSample
lambdaSam
tofSample
armSample
Guide3
armKink2
Guide2
armKink
Guide12
psdGuide1
tofIPulse
tofPulse
PulseShape
PulseShape
tofprePulse
armChoppe
Guide11
psdMod
lambdaMod
tofMod
Moderator
Origin

McStas usage for neutrons



McStas for optimisation



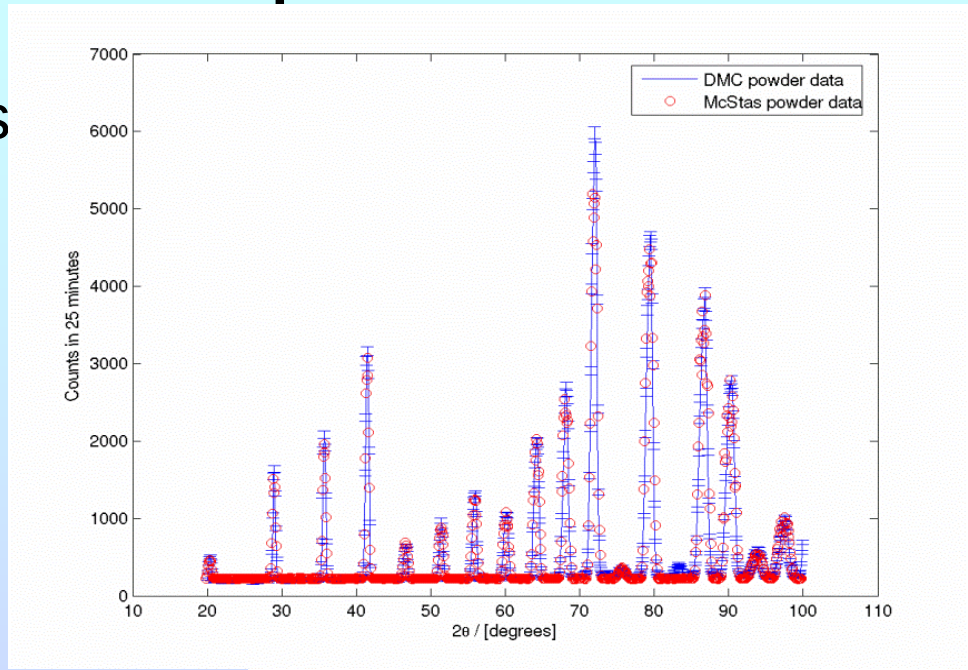


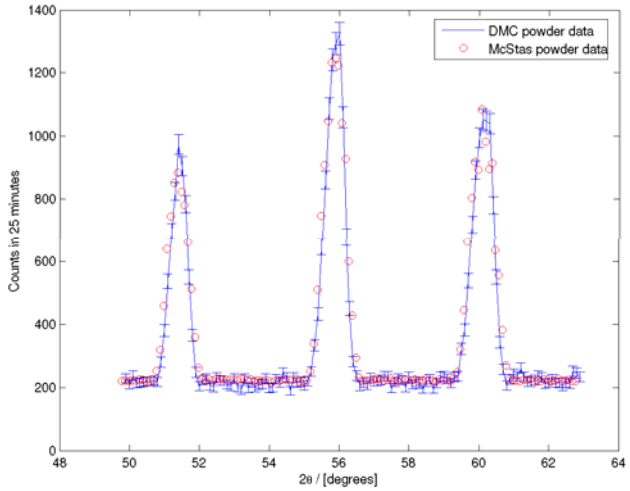
Non-uniform guide coating study, 100 m guides for ESS

Kaspar Klenø, Uni Copenhagen

Tests and cross comparisons

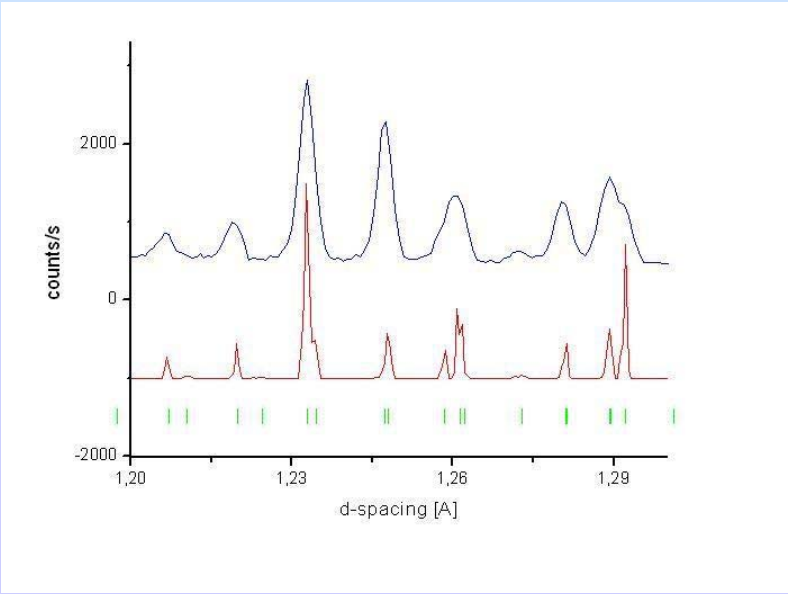
- Much effort has gone into this
  - Here: simulations vs. exp. at powder diffract. DMC, PSI
- The bottom line is
  - McStas agree very well with other packages
  - Experimental line shapes are within 5%
  - Absolute intensities are within 10-30%
- Common understanding:
  - McStas is reliable
  - ... and trusted by the community!





Virtual experiments, definition

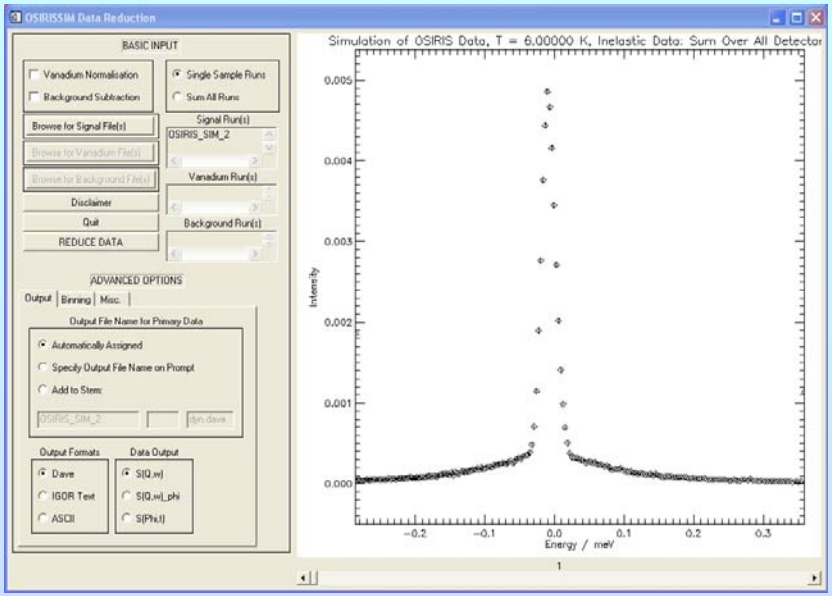
- Simulation of a complete experiment
- … from source to detector
- Controlled like real experiment
- Data analysed by ”real” analysis programs
  - Example: EXED (HMI)
  - New instrument best, compared to existing instrument



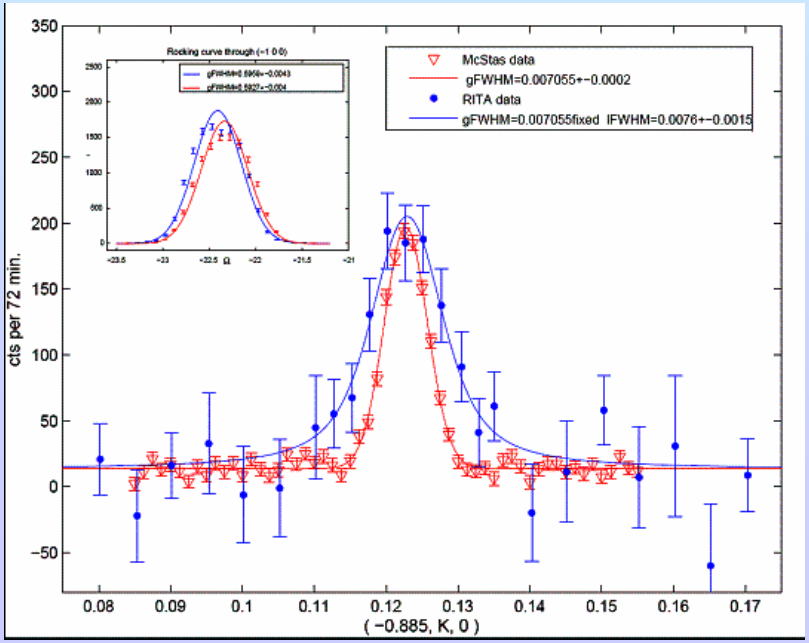
J. Peters, ILL Grenoble

Virtual experiments, analysis

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



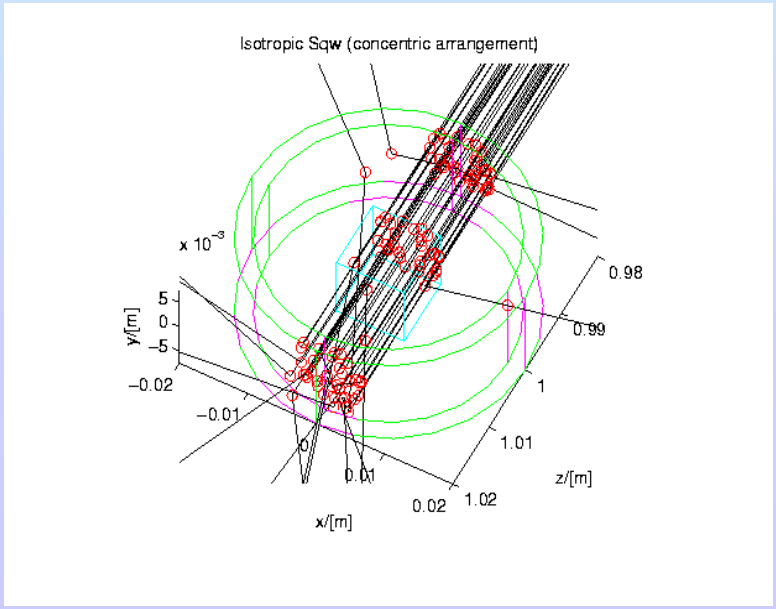
P. Tregenna-Piggott, PSI

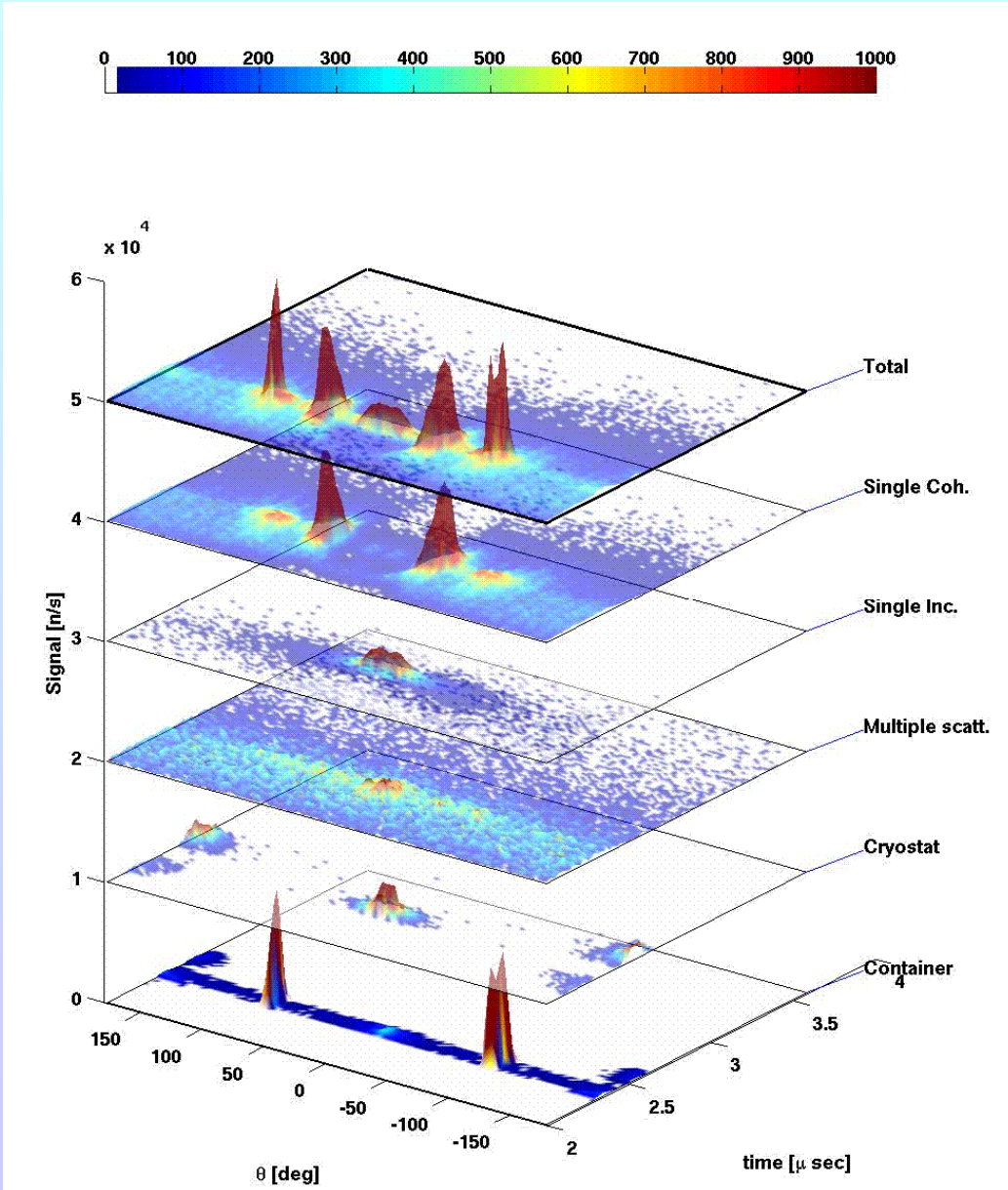


L. Udby, Risø-DTU

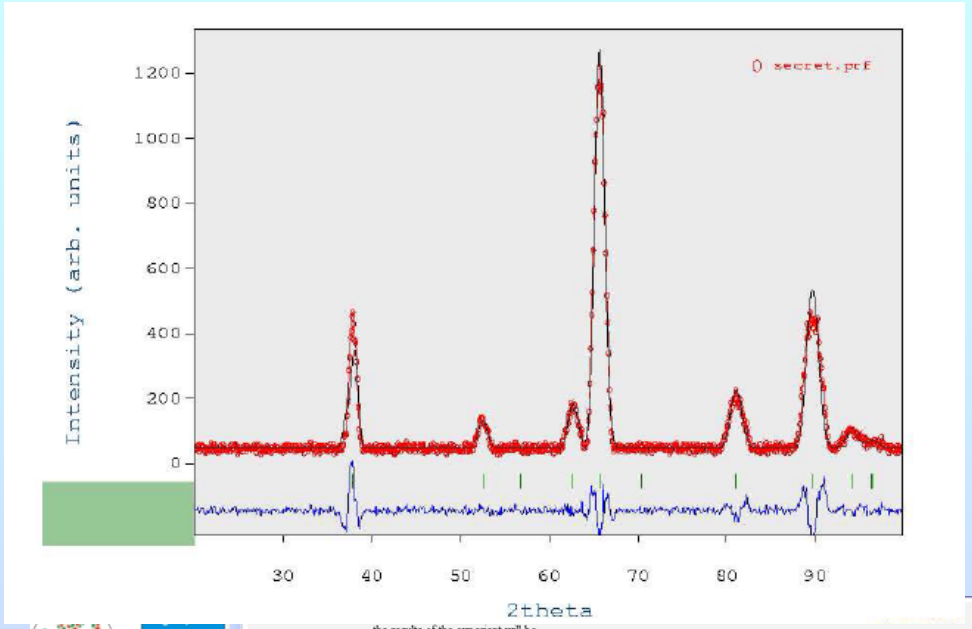
Virtual experiments, analysis

- Virtual TOF exp. at IN6, ILL
  - Liquid Ge sample
  - Coherent / incoherent
  - Multiple scattering
  - And sample environment
- All contributions can be separated by VE !



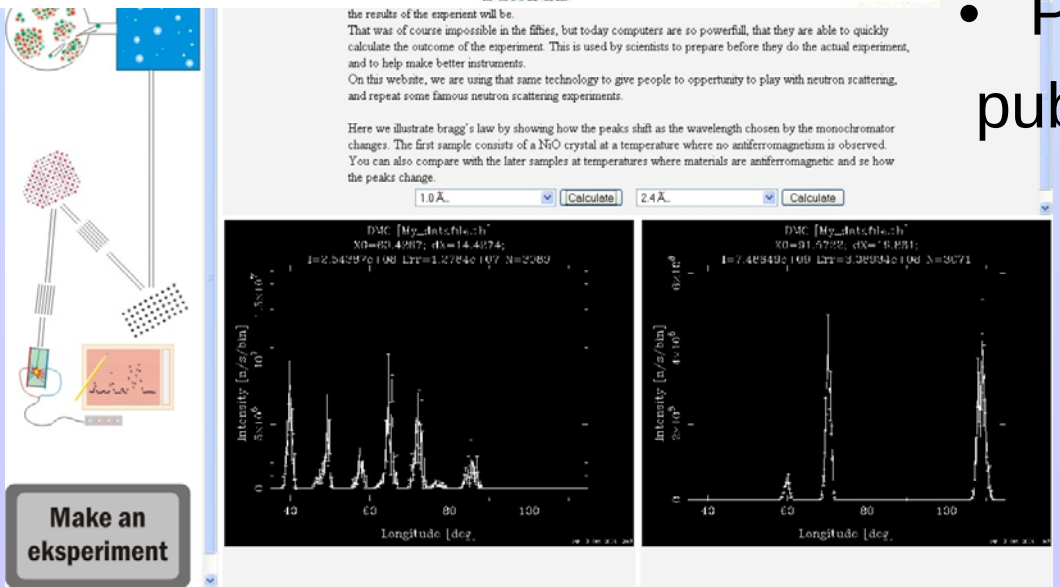


Virtual experiments, teaching etc.



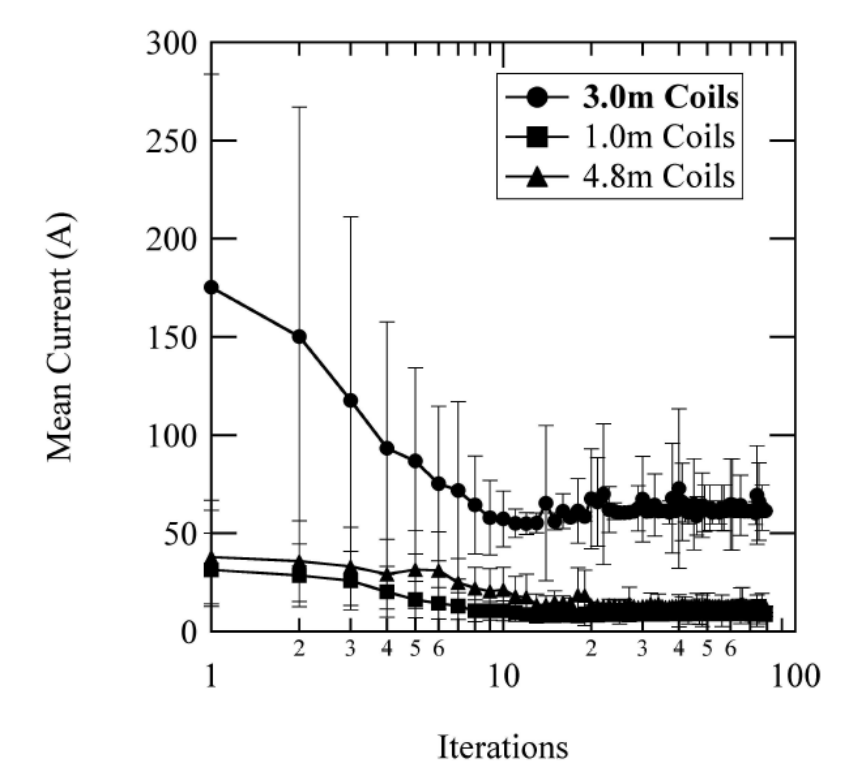
Student team, U. Copenhagen

- Used for university course in Copenhagen (15 students/year)
- ... including full set of teaching notes
- Prototype homepage for public presentation of neutrons



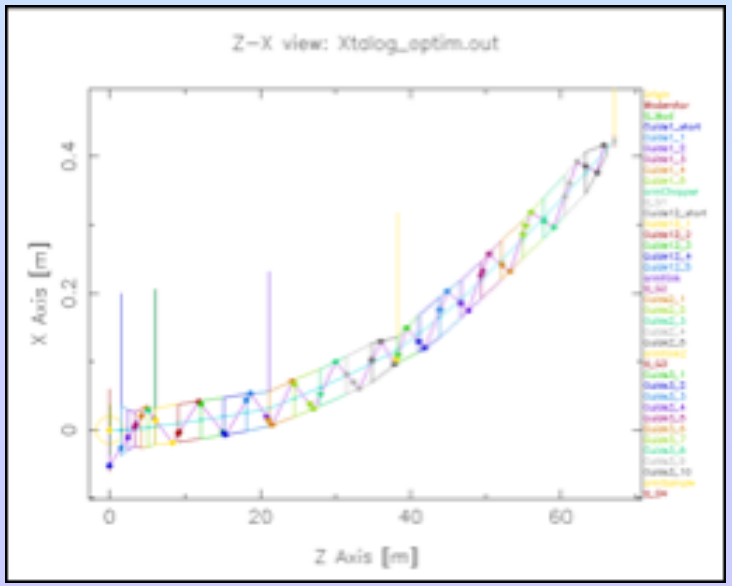
J.O. Birk, K. Klenø, U. Copenhagen

Other features: optimization



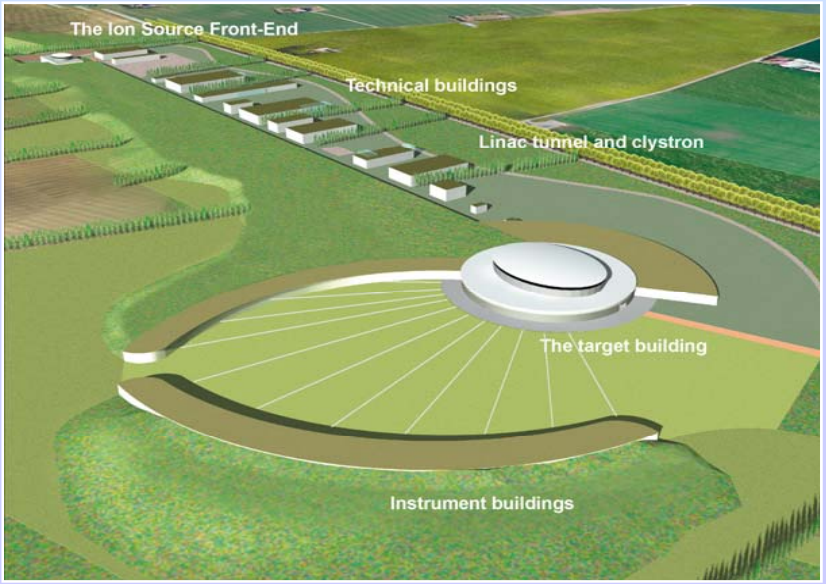
Global optimization of coil currents
P. Bentley, ILL

- Automatic optimization of instruments have been implemented
- Genetic algorithms for large parameter dimensions (>30)



Optimization of guide shape
E. Farhi, ILL

The future neutron spallation sources



- SNS (Oak Ridge) and J_PARC (Tokai): All instruments are simulated by McStas, VITESS, or both

- ESS (S, ES, H ??): McStas is already in use for design

Visions for use of McStas, e.g. at the new spallation sources

- Design instruments
- … using VE on key experiments as benchmarks
- Pre-test of data handling and analysis software (as CERN)
- Evaluate beamtime proposals
- Analyze complex data (e.g. multiple scattering)
- Train students and new users
- Public outreach / PR

- All included in the proposed ESS-Scandinavia budget

Relevance for the X-ray community

- McStas is of great use in neutron instrumentation
  … and will expand to more areas, through VE
- Neutrons and X-rays have much in common
  ... so the step to X-ray simulation is not far

- We will create an X-ray package, McXtrace
  ... using the McStas kernel
  ... and some (modified) components
  ... initially for incoherent radiation only
- 1.1 M€ grant from Danish Research Council
- ESRF is a project partner
  ... In-flow of expertise, interfacing to XOP etc.
- Professor Emeritus Jens Als-Nielsen is contributing
- We will collaborate with all of you
  ... through the open-source philosophy of McStas

- Much more about our ideas, plans and milestones during E Knudsen talk Wednesday at 9:30.

Instrument design

McStas important tool for instrumentdesign at leading neutron sources:

- ILL (FR) IN12, D16, IN5, IN6, D7, D2B, D33, FIGARO, D17,
- ISIS TS2 (UK) LET, CRISP, POLREF, INTER, …
- SNS (US) HYSPEC, SECHOIA, BSS, …
- PSI (CH) FOCUS, MARS, EIGER, RITA-II, …
- J-PARC (JP) “all”