Status of the McStas instrument simulation project

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[5]ESS design update programme, Denmark
[6]ESS design update programme, Switzerland

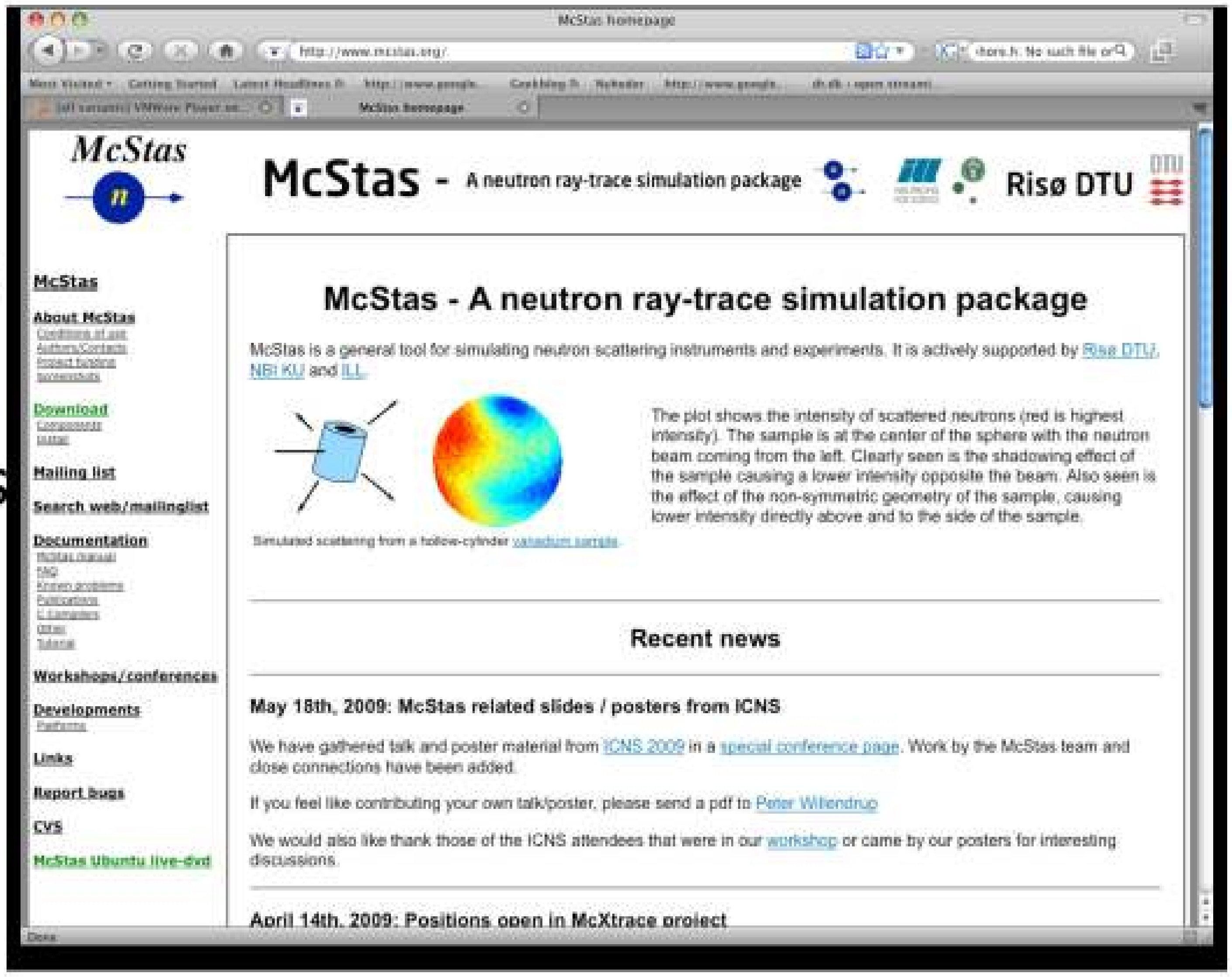
Agenda

- An introduction to
  - McStas
  - Monte Carlo + raytracing
  - Project and technology
- New developments for the **long-awaited** 2.0 release
- Conclusions / lessons learned

McStas Introduction

- Flexible, general simulation utility for neutron scattering experiments.
- Original design for Monte carlo Simulation of triple axis spectrometers
- Developed at DTU Physics, ILL, PSI, Uni CPH
- V. 1.0 by K Nielsen & K Lefmann (1998) RISØ
- Currently 2.5+1 people full time plus students

GNU GPL
license
Open Source



McStas - A neutron ray-trace simulation package

McStas - A neutron ray-trace simulation package

McStas is a general tool for simulating neutron scattering instruments and experiments. It is actively supported by Risø DTU, NBI KU and ILL.

Simulated scattering from a hollow-cylinder vanadium sample.

The plot shows the intensity of scattered neutrons (red is highest intensity). The sample is at the center of the sphere with the neutron beam coming from the left. Clearly seen is the shadowing effect of the sample causing a lower intensity opposite the beam. Also seen is the effect of the non-symmetric geometry of the sample, causing lower intensity directly above and to the side of the sample.

Recent news

May 18th, 2009: McStas related slides / posters from ICNS

We have gathered talk and poster material from ICNS 2009 in a special conference page. Work by the McStas team and close connections have been added.

If you feel like contributing your own talk/poster, please send a pdf to Peter Willendrup

We would also like thank those of the ICNS attendees that were in our workshop or came by our posters for interesting discussions.

April 14th, 2009: Positions open in McXtrace project

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

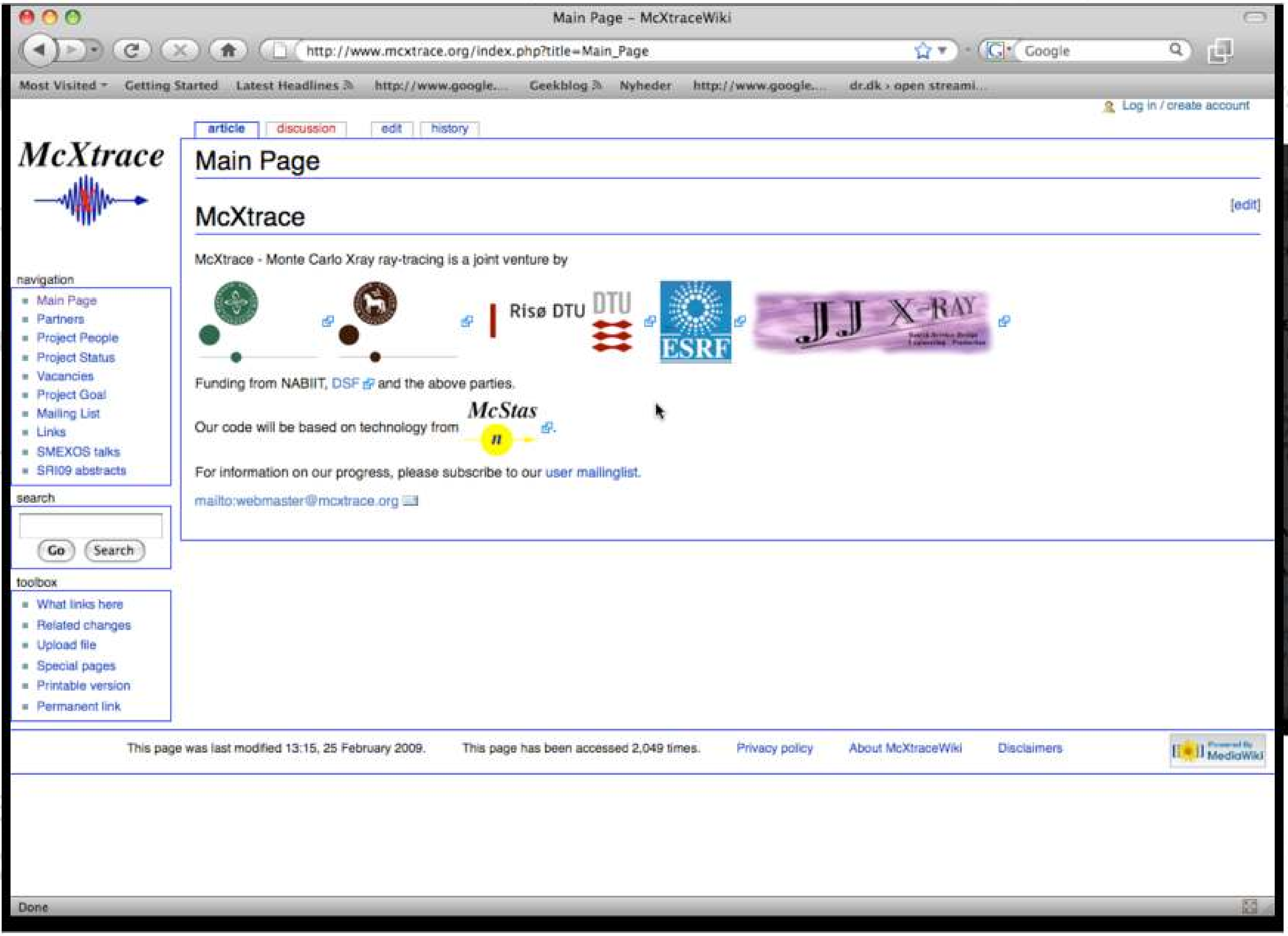
mcstas-users@mcstas.org mailinglist

See E. Knudsen poster!

McStas Introduction

McXtrace - since jan 2009 similar in X-rays

- Flexible, general simulation utility for neutron scattering experiments.
- Origina
- Develop
- V. 1.0 b
- Current



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Main Page

McXtrace

[edit]

McXtrace - Monte Carlo Xray ray-tracing is a joint venture by

Risø DTU DTU ESRF JJ X-RAY

Funding from NABIIT, DSF and the above parties.

Our code will be based on technology from McStas.

For information on our progress, please subscribe to our user mailinglist.

mailto:webmaster@mcxtrace.org

This page was last modified 13:15, 25 February 2009. This page has been accessed 2,049 times. Privacy policy About McXtraceWiki Disclaimers

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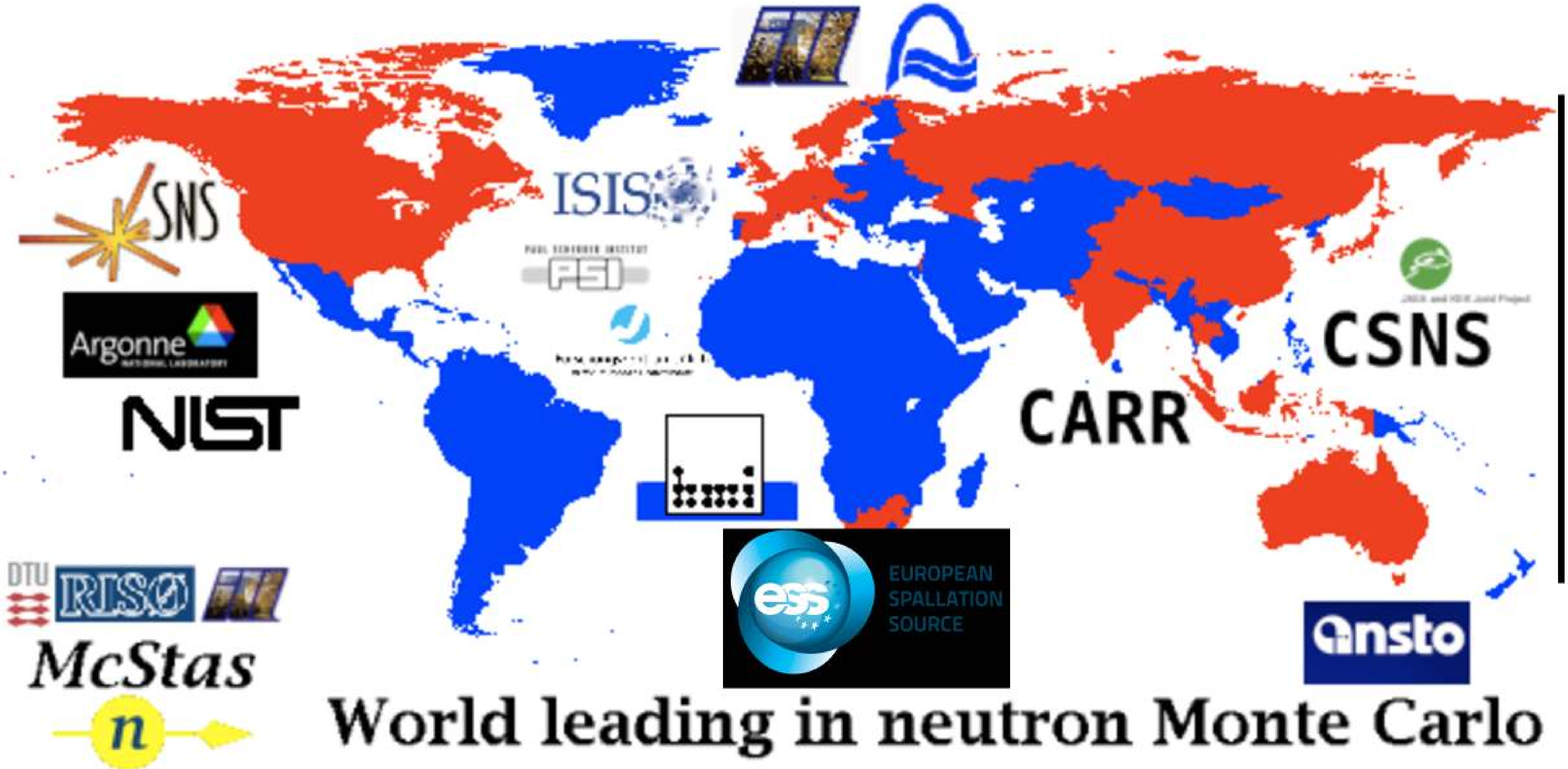
Proje
http

ist

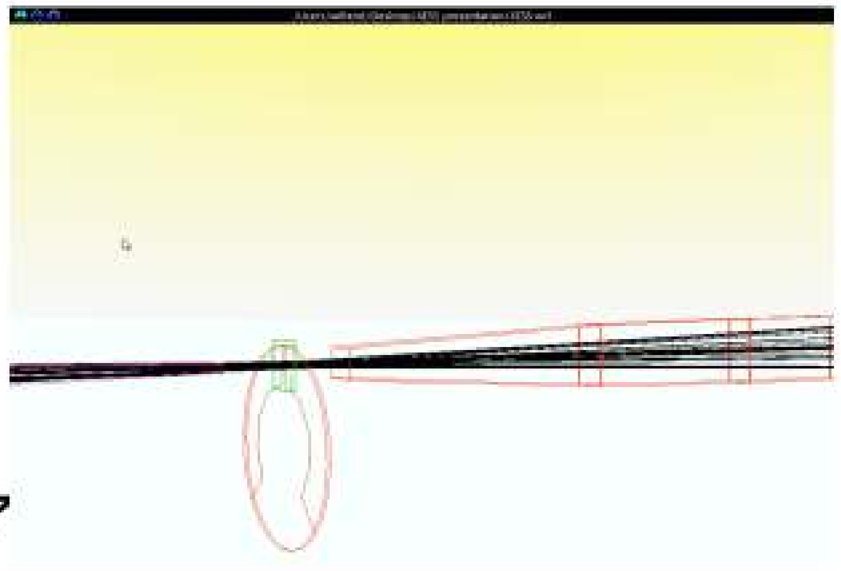
- Synergy, knowledge transfer, shared infrastructure

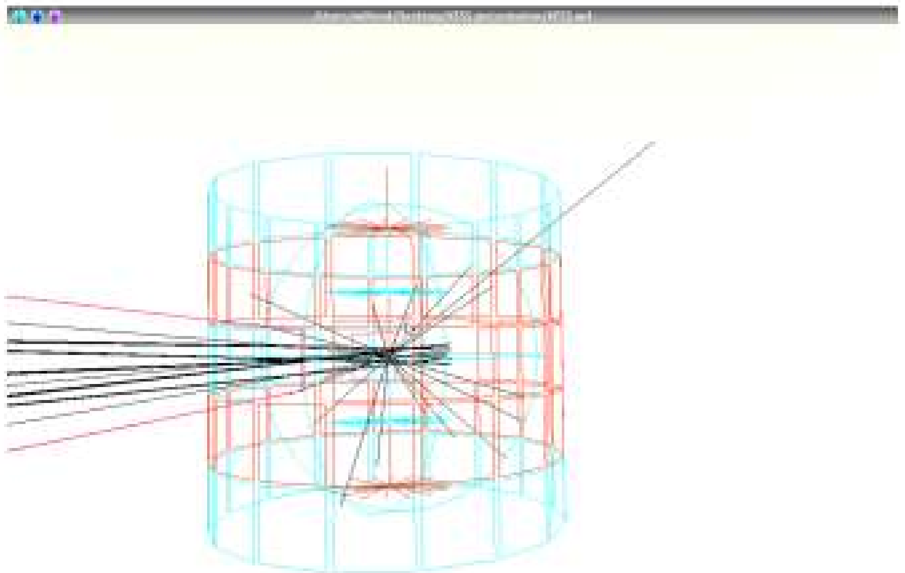
McStas Introduction

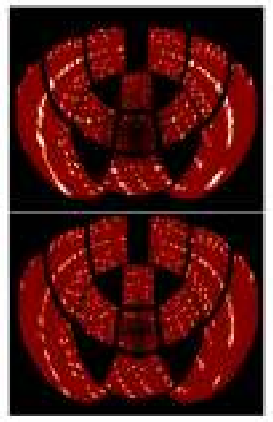


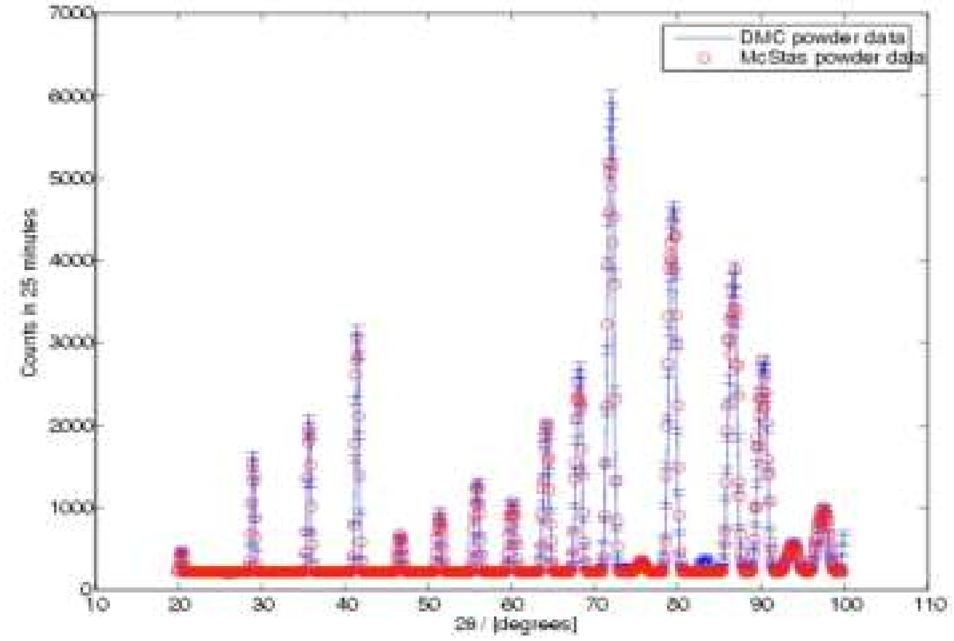
World leading in neutron Monte Carlo

What is McStas used for?



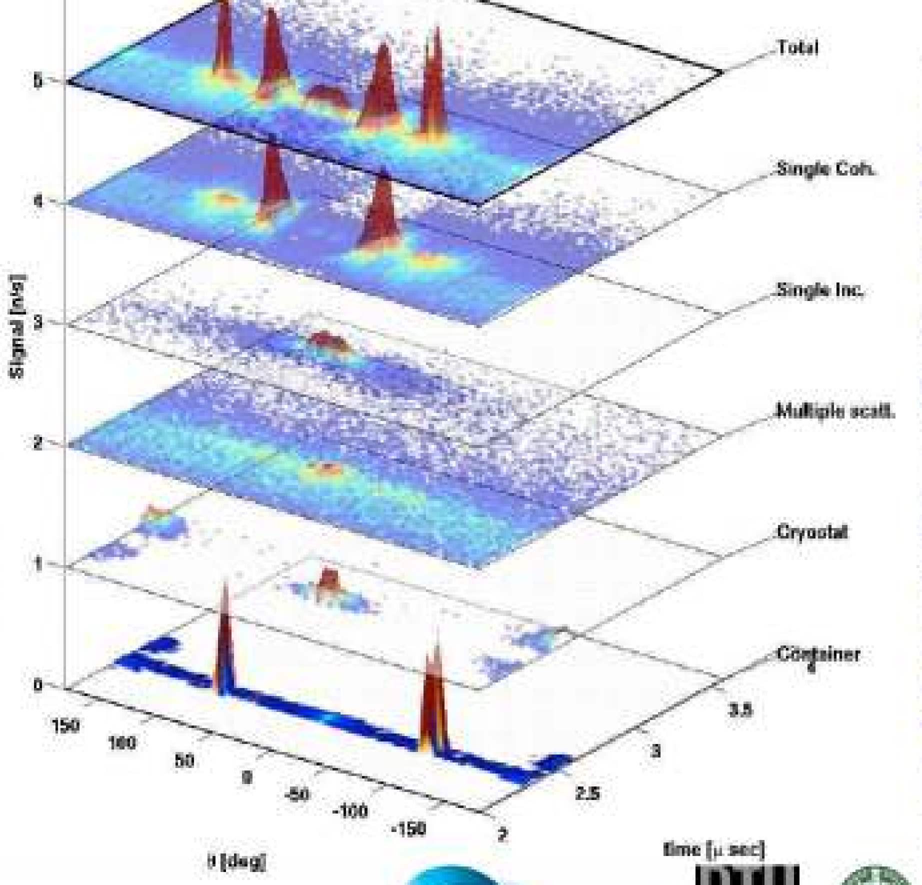


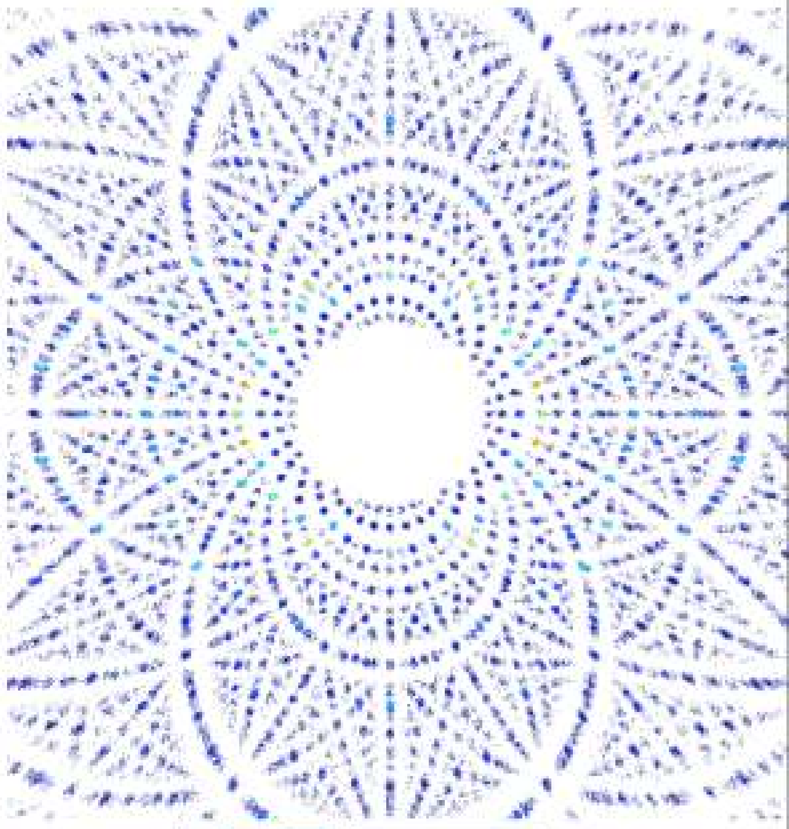


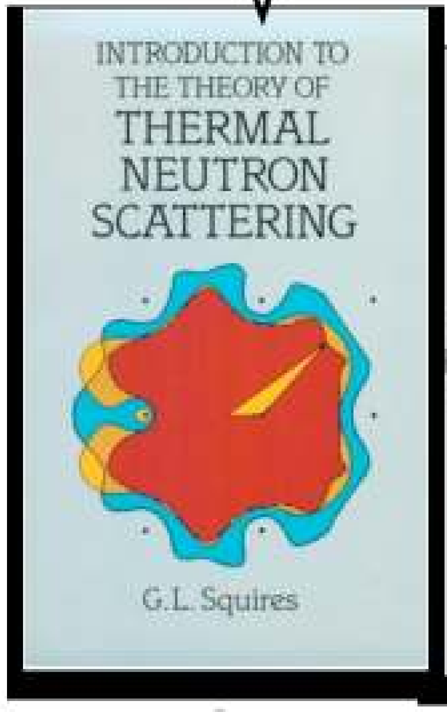


- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

KU, DTU 2005-2012
INSIS, NIDS, ESS workshops

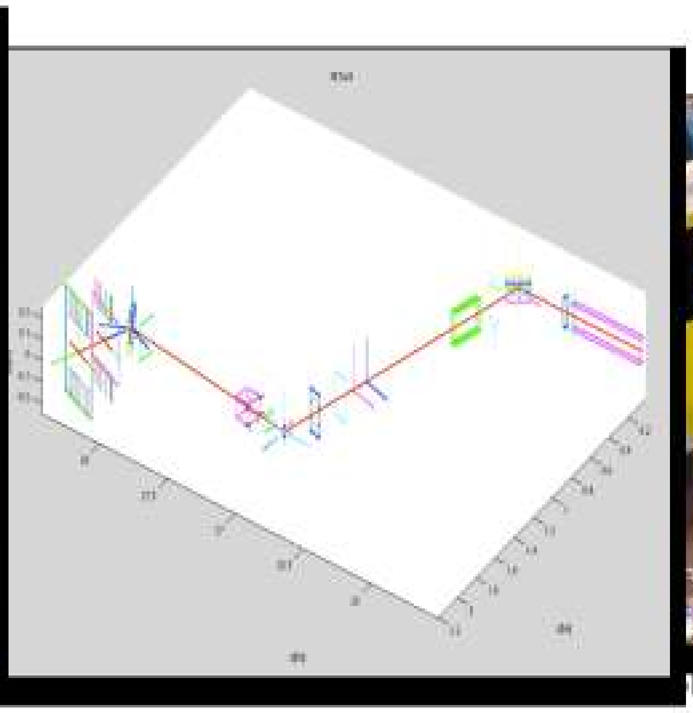






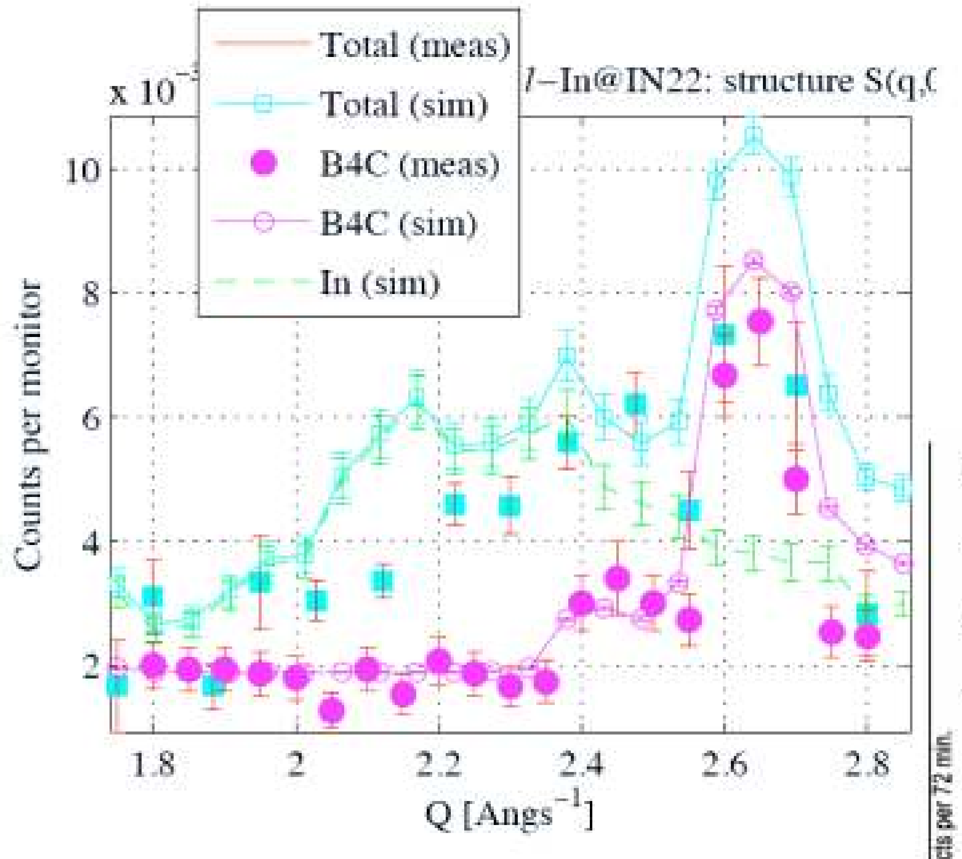
INTRODUCTION TO THE THEORY OF THERMAL NEUTRON SCATTERING

G.L. Squires

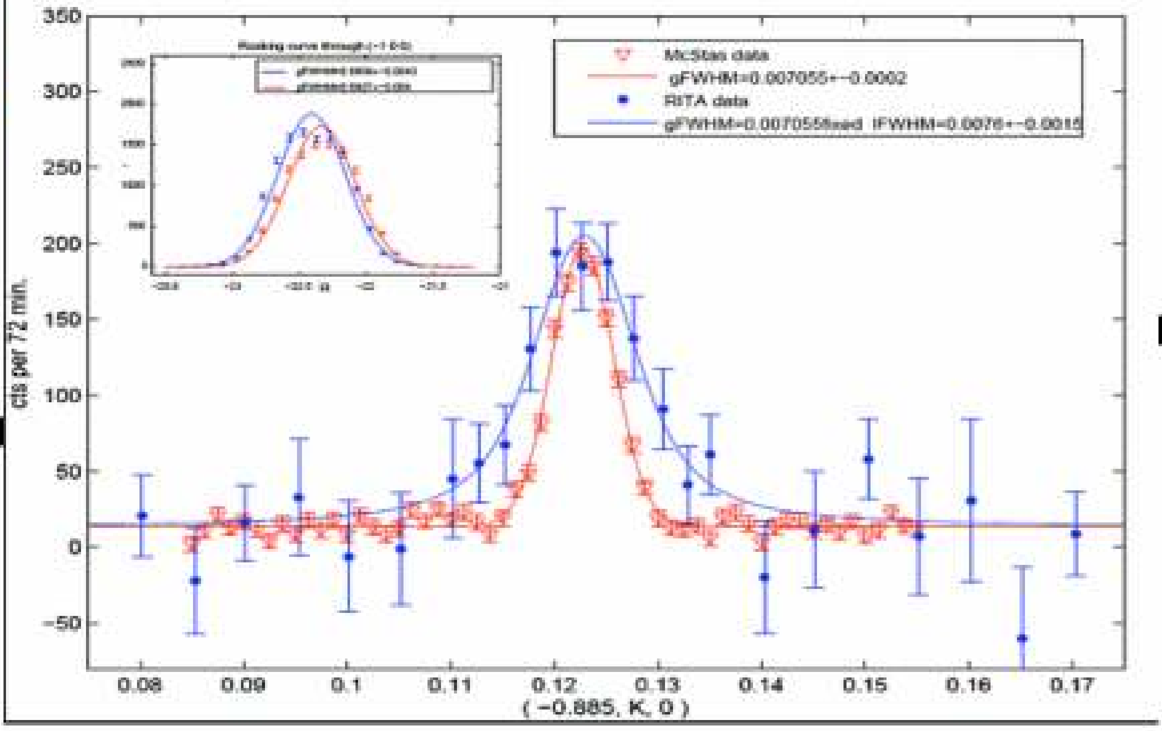


Reliability - cross comparisons

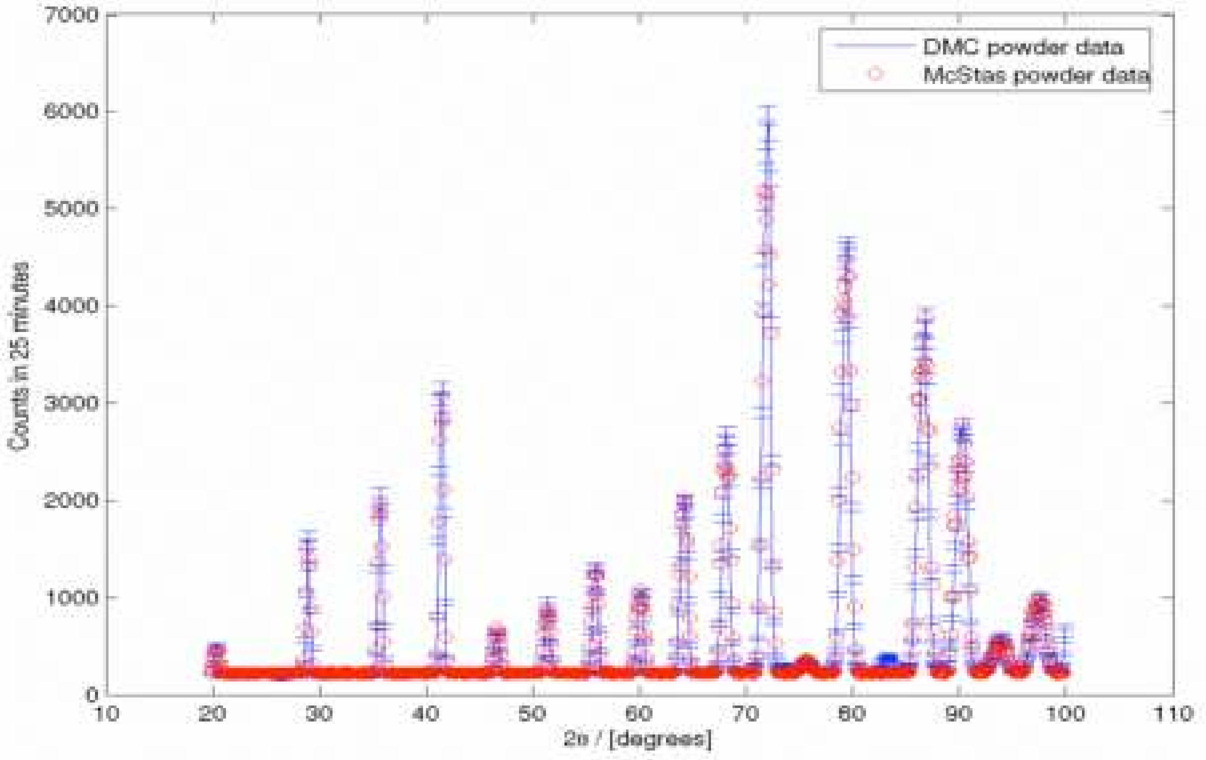
- Much effort has gone into this
- Here: simulations vs. exp. at powder diffract. DMC, PSI
- The bottom line is
- McStas agree very well with other packages (NISP, Vitess, IDEAS, RESTRAX, ...)
- Experimental line shapes are within 5%
- Absolute intensities are within 10%
- Common understanding: McStas and similar codes are reliable



E. Farhi, P. Willendrup et al., in



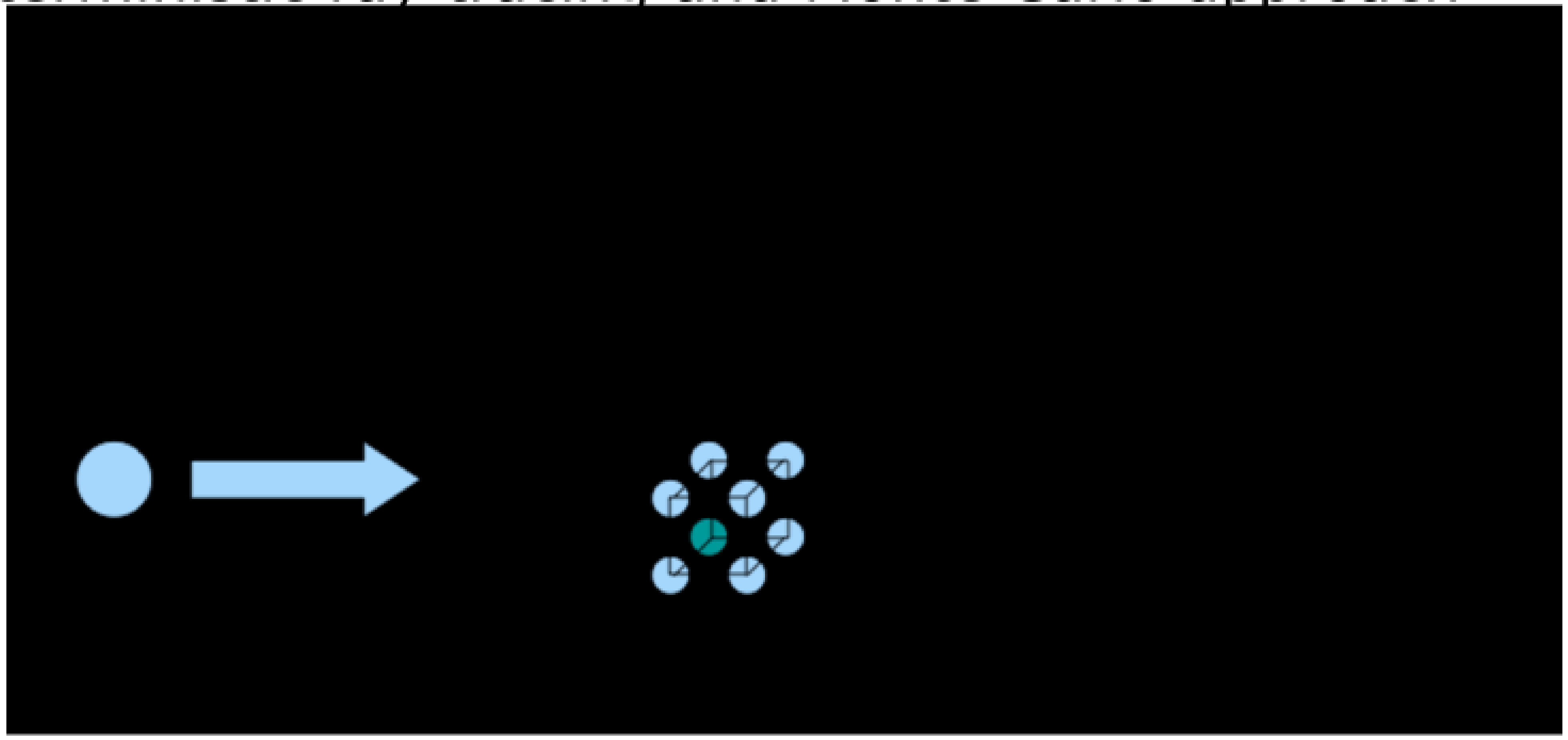
L. Udby, NIMA 2011, Volume 634 (2011)



P. Willendrup et al., Physica B, 386, (2006),

Elements of Monte-Carlo raytracing

- Instrument Monte Carlo methods implement coherent scattering effects
- Uses deterministic propagation where this can be done
- Uses Monte Carlo sampling of “complicated” distributions and stochastic processes and multiple outcomes with known probabilities are involved
- - I.e. inside scattering matter
- Uses the particle-wave duality of the neutron to switch back and forward between deterministic ray tracing and Monte Carlo approach

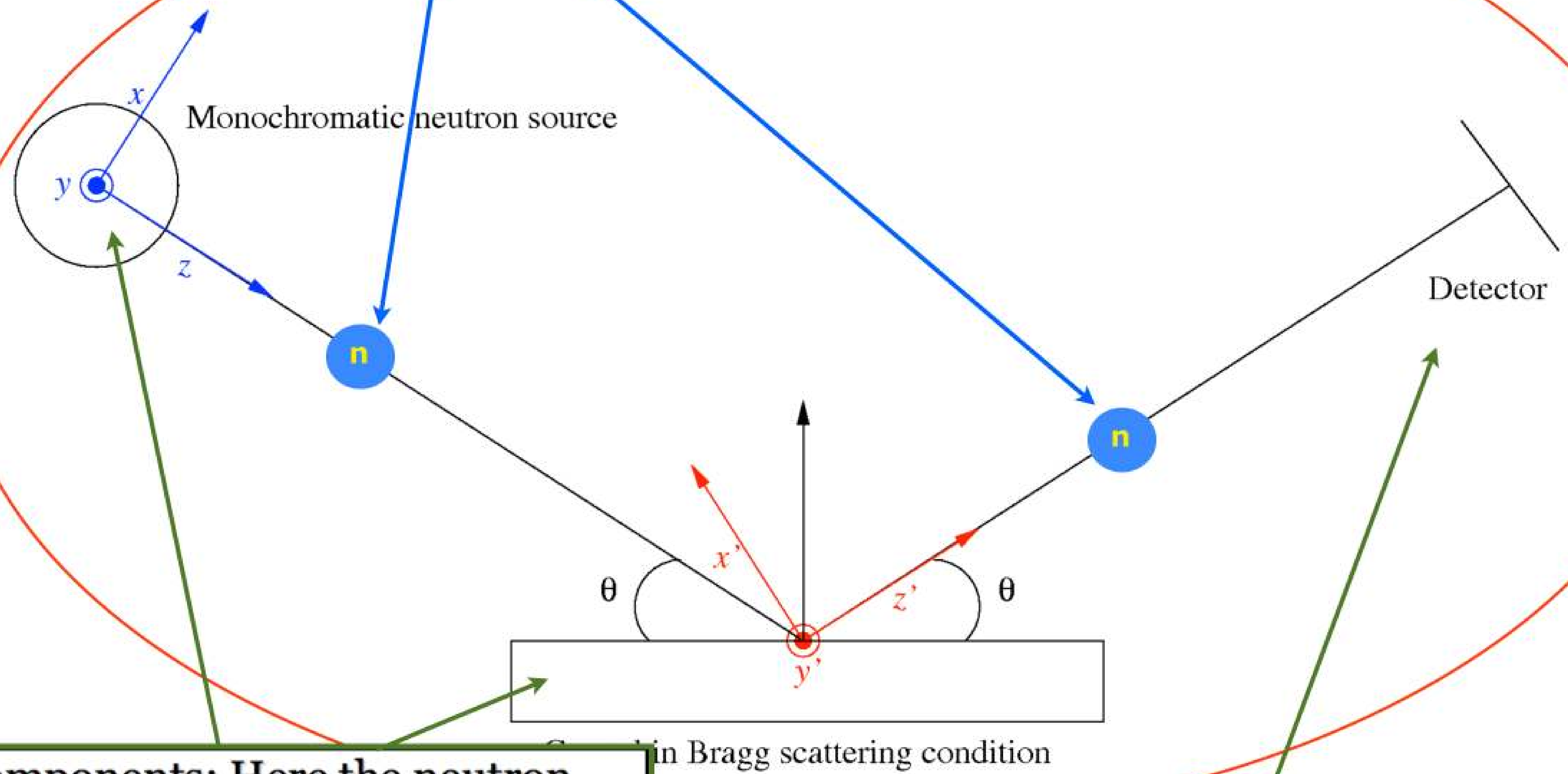


- Result: A realistic and efficient transport of neutrons in the thermal and cold range

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)
Time (t)

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



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

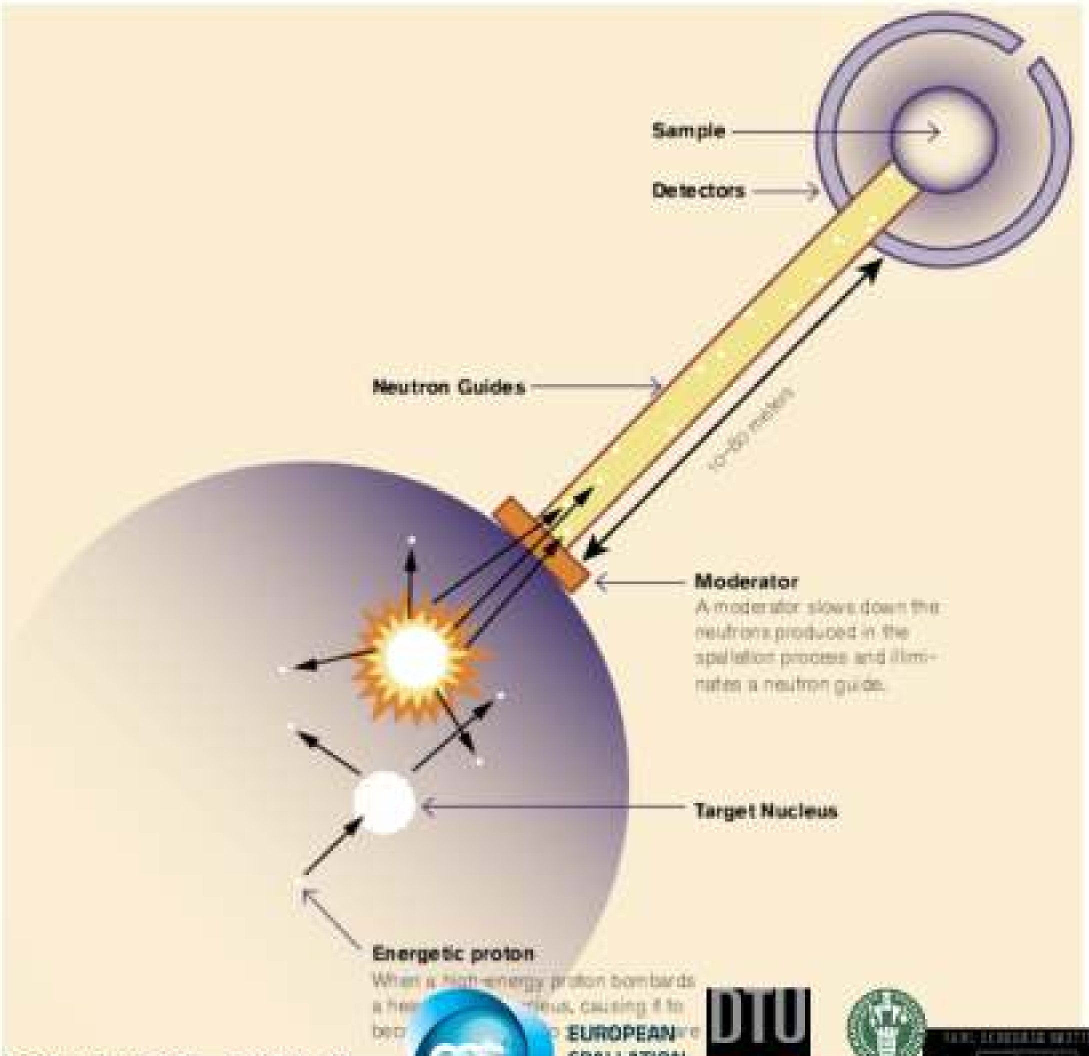
Local, internal coordinate system!

McStas overview

- Portable code (Unix/Linux/Mac/Windoze)

- Ran on everything from iPhone to 1000+ node cluster!

- 'Component' files (~100) inserted from library
  - Sources
  - Optics
  - Samples
  - Monitors
  - If needed, write your own comps


Sample
Detectors
Neutron Guides
10–80 meters
Moderator
A moderator slows down the neutrons produced in the spallation process and illuminates a neutron guide.
Target Nucleus
Energetic proton
When a high-energy proton bombards a hea[illegible] nucleus, causing it to bec[illegible]

- DSL + ISO-C code gen.

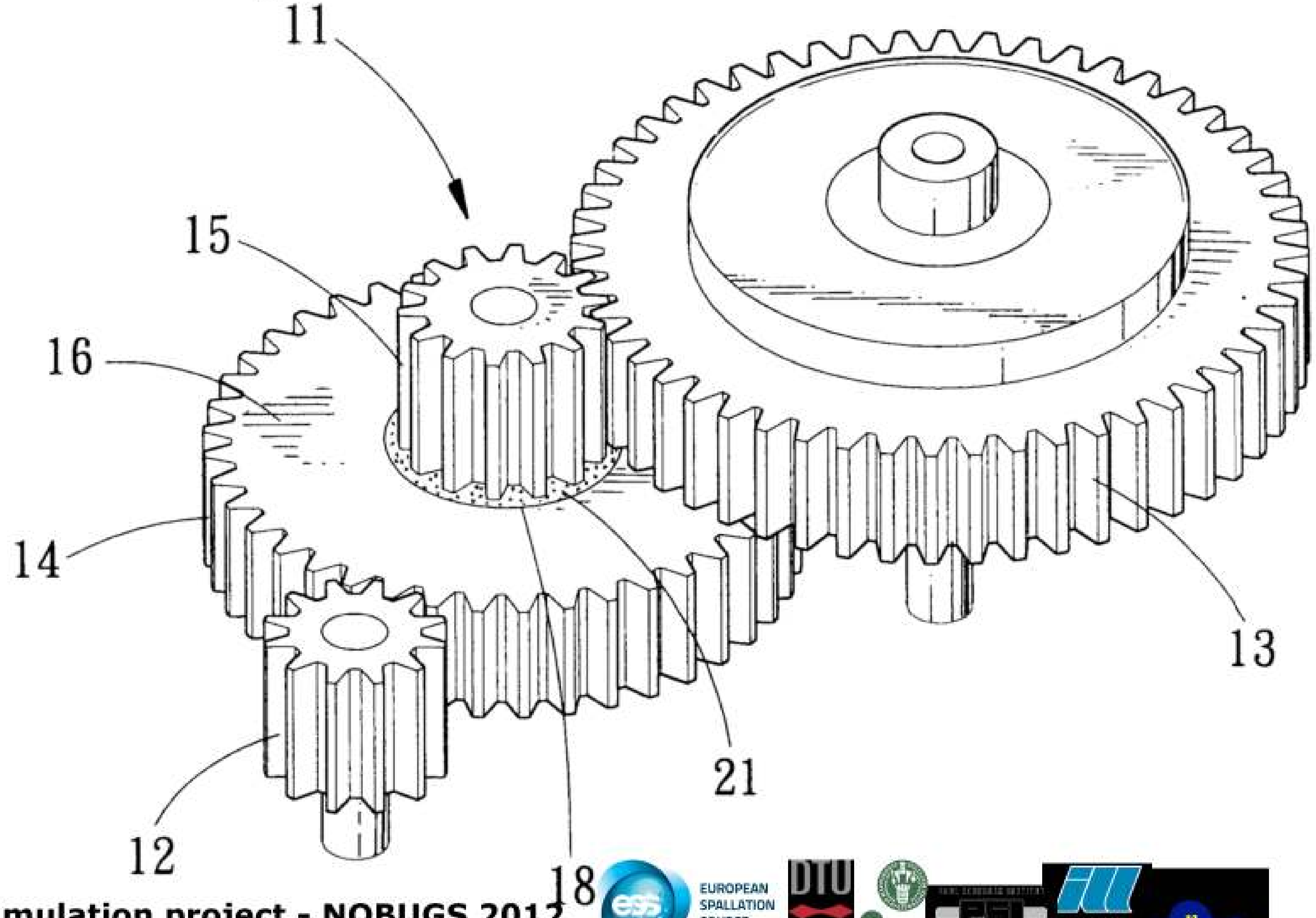
International Organization for Standardization

Under-the-hood / inner workings

- Domain-specific-language (DSL) based on compiler technology (LeX+Yacc)
  - Simple Instrument language $\xrightarrow{\text{Code generation}}$ ISO C

International Organization for Standardization

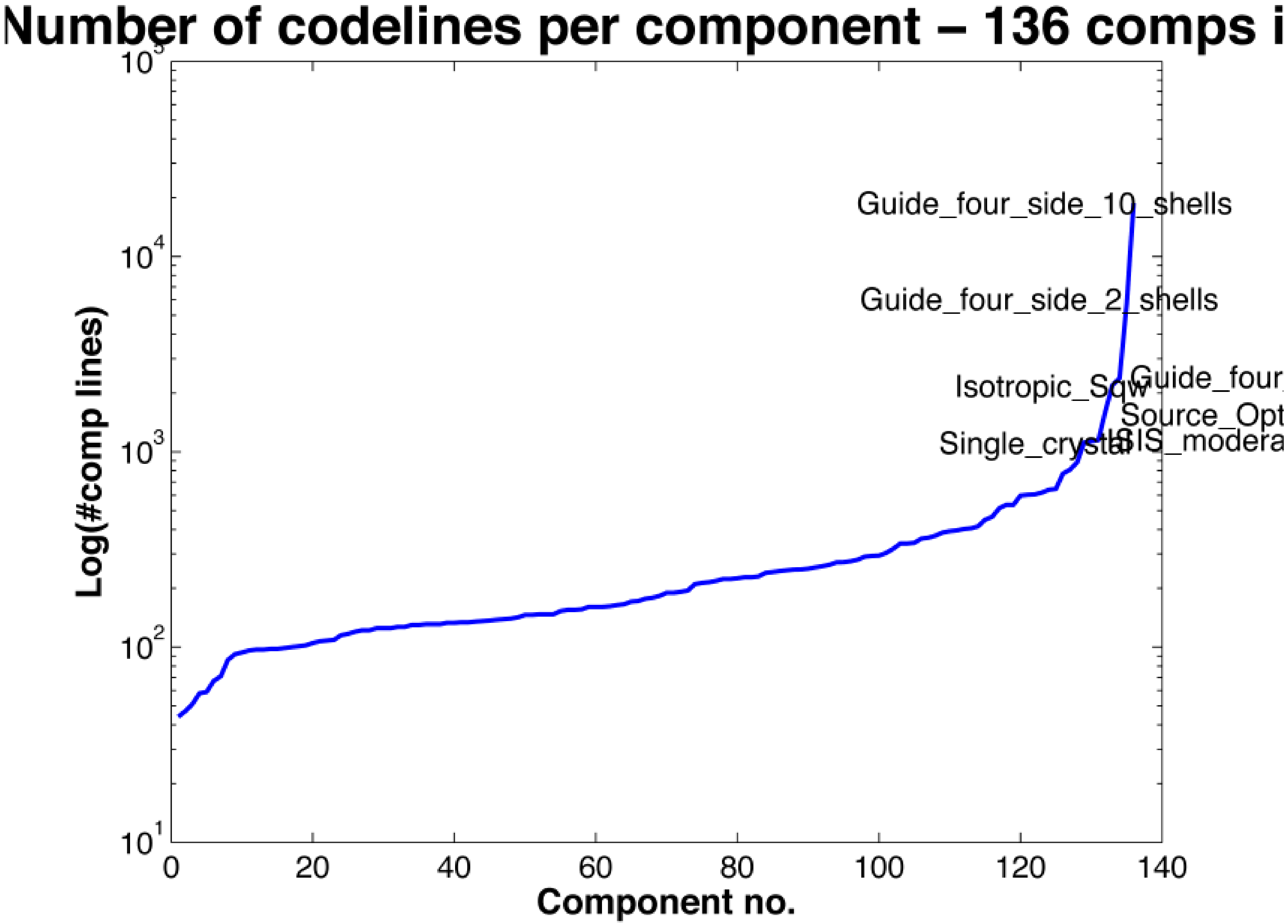
- Component codes realizing beamline parts (including user contribs)
- Library of common functions for e.g.
  - I/O
  - Random numbers
  - Physical constants
  - Propagation
  - Precession in fields
  - ...



EUROPEAN SPALLATION SOURCE

Writing/modifying comps is not complex...

- Most comps are quite simple and short ~ 100 lines
- 30-40% of existing and new additions are from users
- Requirement: Test-scenario for documentation & unit test



Syntax in one, complex view...

```
{SPLIT} COMPONENT name = comp(parameters) {WHEN condition}
  AT (...) [RELATIVE [reference|PREVIOUS] | ABSOLUTE]
  {ROTATED {RELATIVE [reference|PREVIOUS] | ABSOLUTE} }
  {GROUP group_name}
  {EXTEND C_code}
  {JUMP [reference|PREVIOUS|MYSELF|NEXT] [ITERATE number_of_times | WHEN
condition] }
```

DECLARE / INITIALIZE

- Full flexibility of C in your instrumentfile!

- Use the DECLARE section define user variables and functions.
  - DECLARE %{
  -    double myvar;
  - %}

- Use INITIALIZE for initialization of user variables and calculations.
  - INITIALIZE %{
  -    myvar = sqrt(PI*input_var)*rand01();
  - %}

- - Both use normal c-syntax.

K & R

SEGUNDA EDICION

Con base en el ANSI C

EL LENGUAJE DE PROGRAMACION C

BRIAN W. KERNIGHAN
DENNIS M. RITCHIE

- BEWARE: (example) What you do in the c-style areas is c-standard, e.g. trigonometric functions from math.h use radians! - McStas placement specifiers work in degrees, etc...

International Organization for Standardization

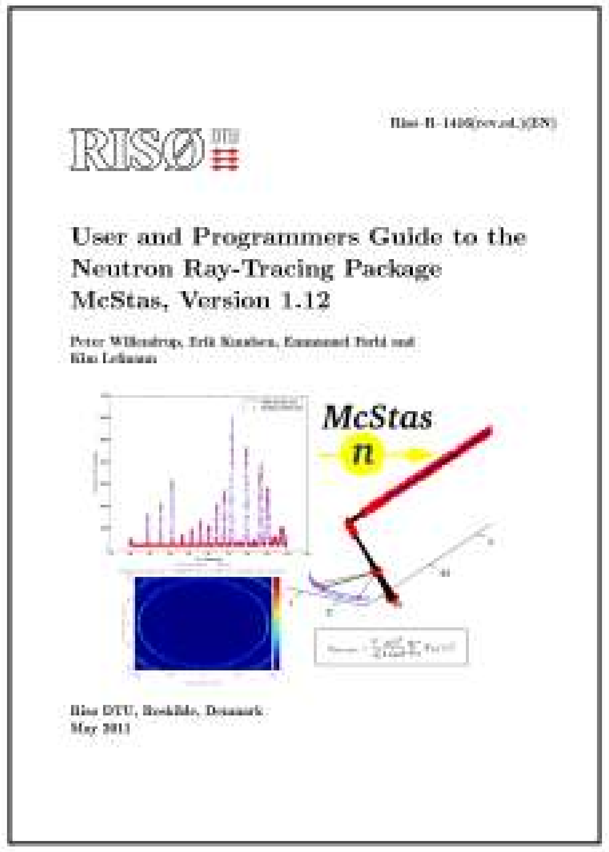
Documentation

- Basic use info is available inside comp & instr codes, extracted by perl to html

- 100+ page manuals documenting
  - Metalanguage
  - What is "under the hood"
  - Examples of practical use plus advanced features
  - Assumptions and algorithms applied in the components

- More than 70 example instruments

- Various tutorial and teach yourself solutions are available



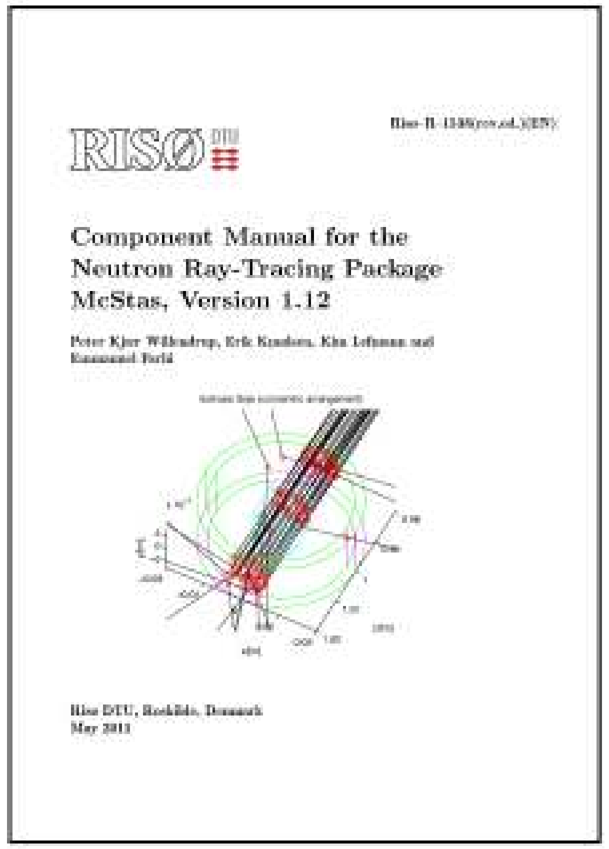
RISØ DTU

Risø-R-1416(rev.ed.)(EN)

User and Programmers Guide to the Neutron Ray-Tracing Package McStas, Version 1.12

Peter Willendrup, Erik Knudsen, Emmanuel Farhi and Kim Lefmann

Risø DTU, Roskilde, Denmark
May 2011



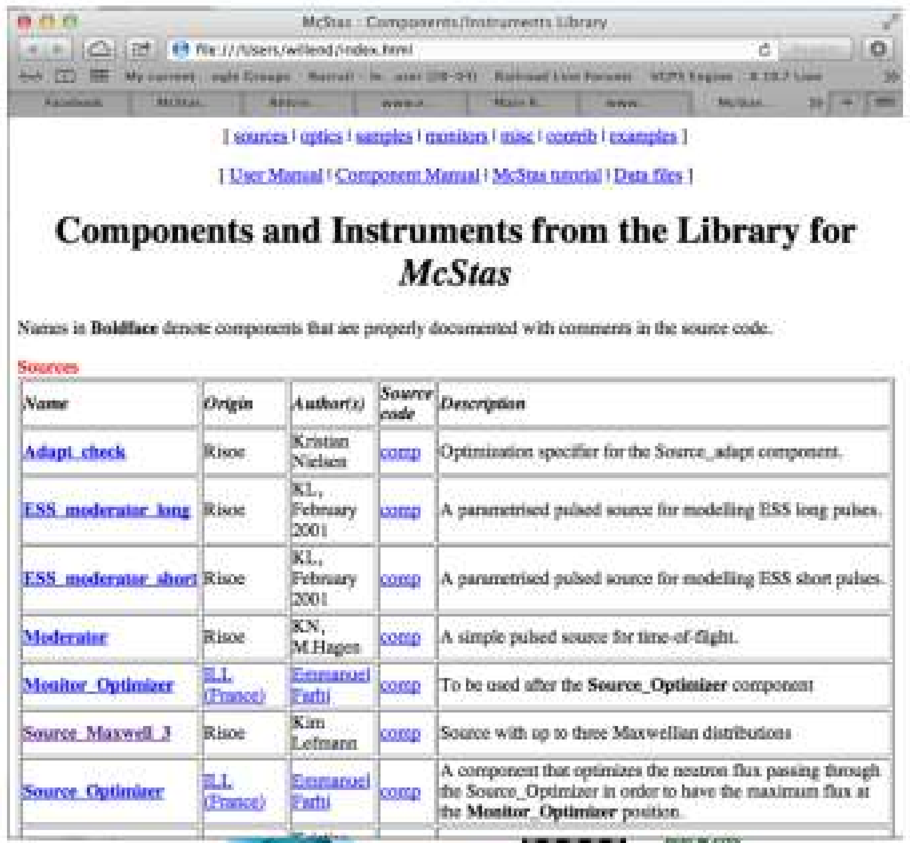
RISØ DTU

Risø-R-1538(rev.ed.)(EN)

Component Manual for the Neutron Ray-Tracing Package McStas, Version 1.12

Peter Kjær Willendrup, Erik Knudsen, Kim Lefmann and Emmanuel Farhi

Risø DTU, Roskilde, Denmark
May 2011



McStas : Components/Instruments Library
file:///Users/willend/index.html

[sources | optics | samples | monitors | misc | contrib | examples]

[User Manual | Component Manual | McStas tutorial | Data files]

Components and Instruments from the Library for *McStas*

Names in **Boldface** denote components that are properly documented with comments in the source code.

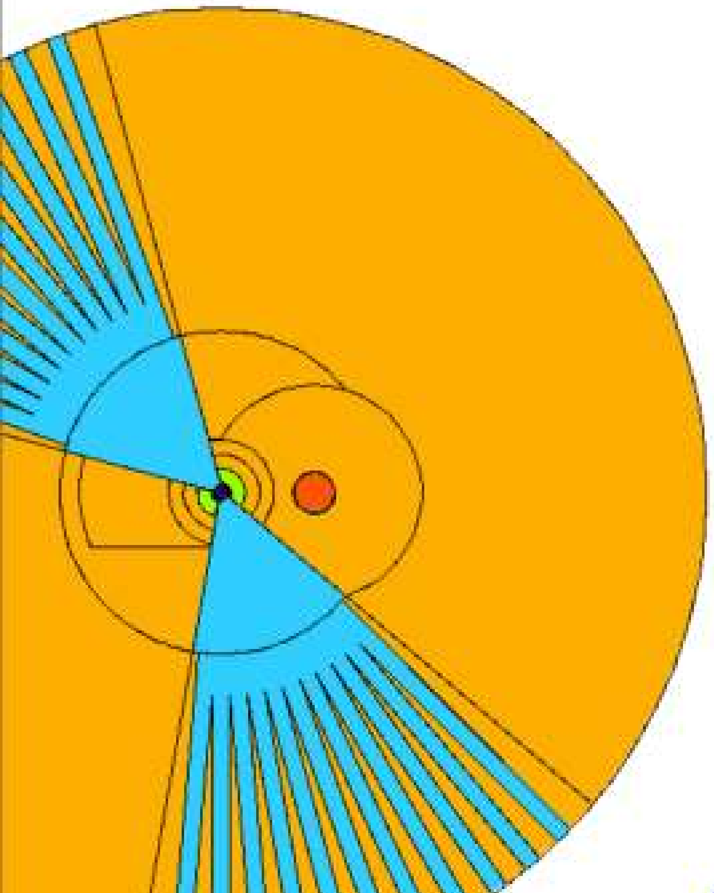
Sources

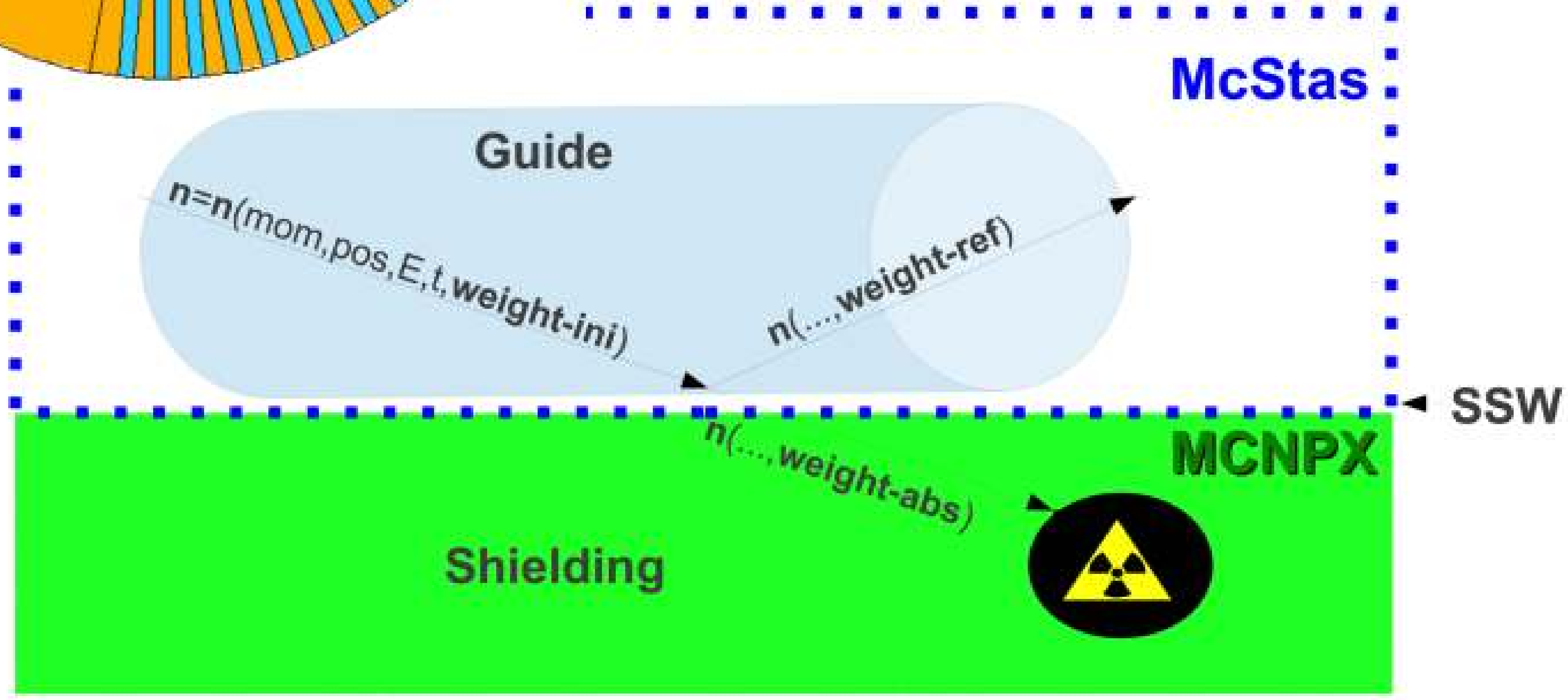
Name	*Origin*	*Author(s)*	*Source code*	*Description*
Adapt_check	Risoe	Kristian Nielsen	comp	Optimization specifier for the Source_adapt component.
ESS_moderator_long	Risoe	KL, February 2001	comp	A parametrised pulsed source for modelling ESS long pulses.
ESS_moderator_short	Risoe	KL, February 2001	comp	A parametrised pulsed source for modelling ESS short pulses.
Moderator	Risoe	KN, M.Hagen	comp	A simple pulsed source for time-of-flight.
Monitor_Optimizer	ILL (France)	Emmanuel Farhi	comp	To be used after the **Source_Optimizer** component
Source_Maxwell_3	Risoe	Kim Lefmann	comp	Source with up to three Maxwellian distributions
Source_Optimizer	ILL (France)	Emmanuel Farhi	comp	A component that optimizes the neutron flux passing through the Source_Optimizer in order to have the maximum flux at the **Monitor_Optimizer** position.

New developments 1 - work on McStas-MCNPX interfaces

The task:

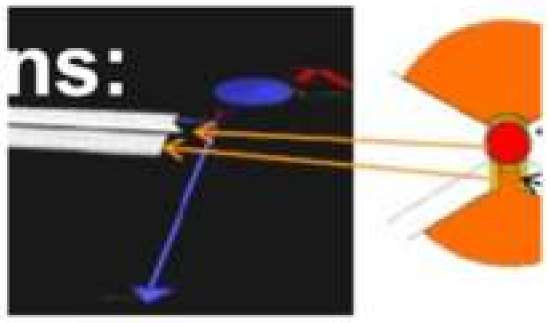
"Interfacing the MCNP and McStas Monte Carlo codes for improved optimization of the ESS moderator-beam extraction systems"



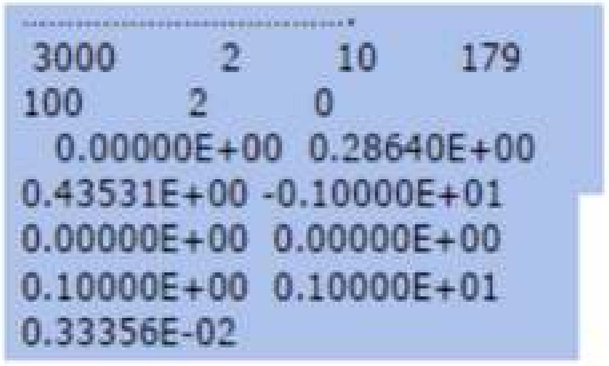


The solutions:

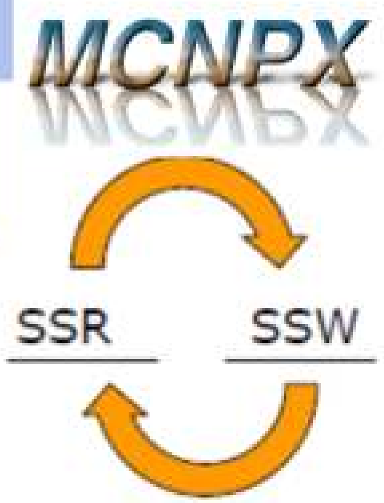
- Tally



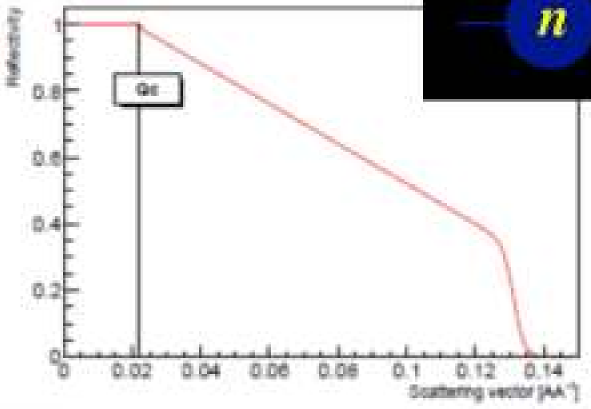
- Ptrac



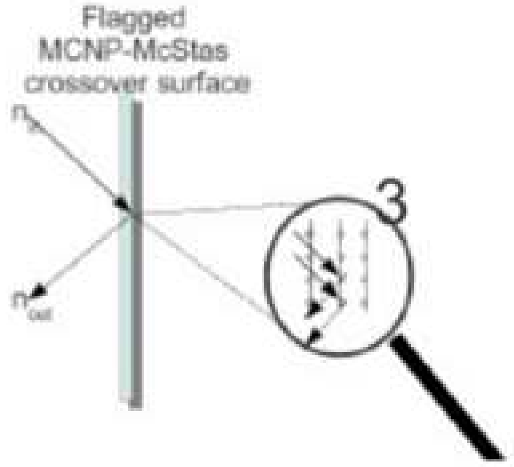
```
 3000       2      10      179
100       2       0
   0.00000E+00  0.28640E+00
0.43531E+00 -0.10000E+01
0.00000E+00  0.00000E+00
0.10000E+00  0.10000E+01
0.33356E-02
```



- SSW
- Supermirror



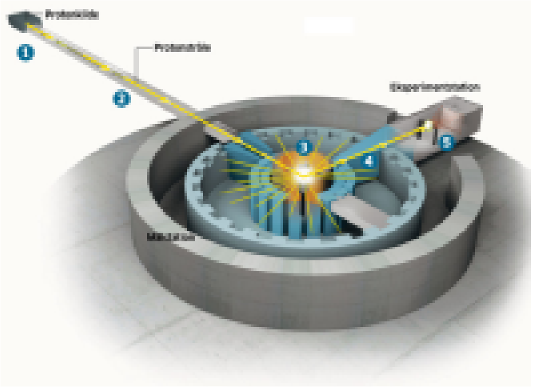
- Compile



S 2012

New developments 2 - New Python-based tools and web frontend

See J. Brinch poster



Neutron simulations from the web

Johan Brinch[1], Peter Willendrup[1], Emmanuel Farhi[2]

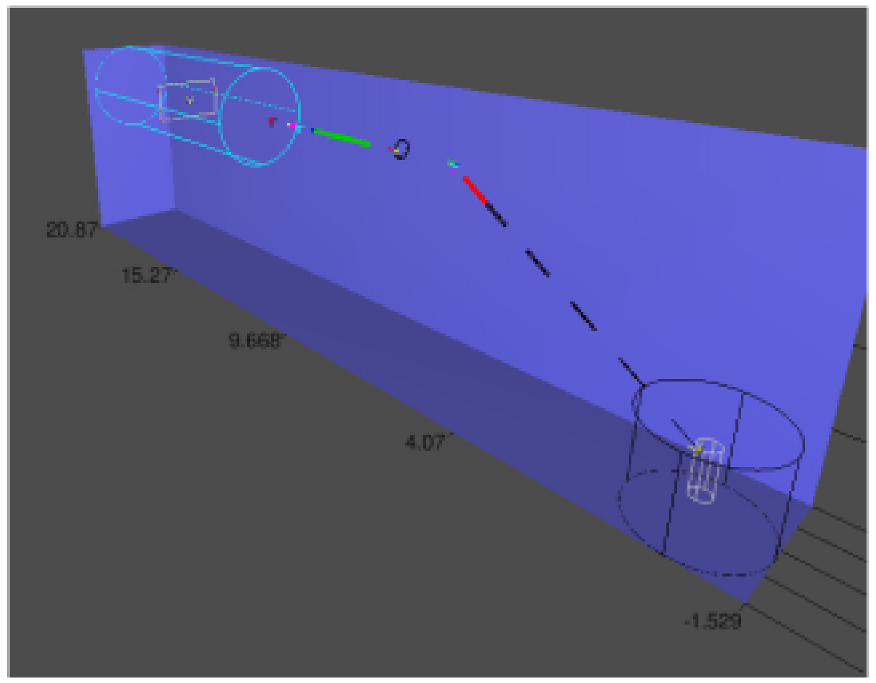
1. Physics Department, Technical University of Denmark; {JSBN,PKWI}@FYSIK.DTU.DK
2. Institut Laue-Langevin, Grenoble, France

McStas

Overview

McStas is developing a web-interface for the simulation software, based on HTML and Javascript. The web-interface allows a user to run the McStas simulation software from a server; without installing it herself.

3D Visualisation



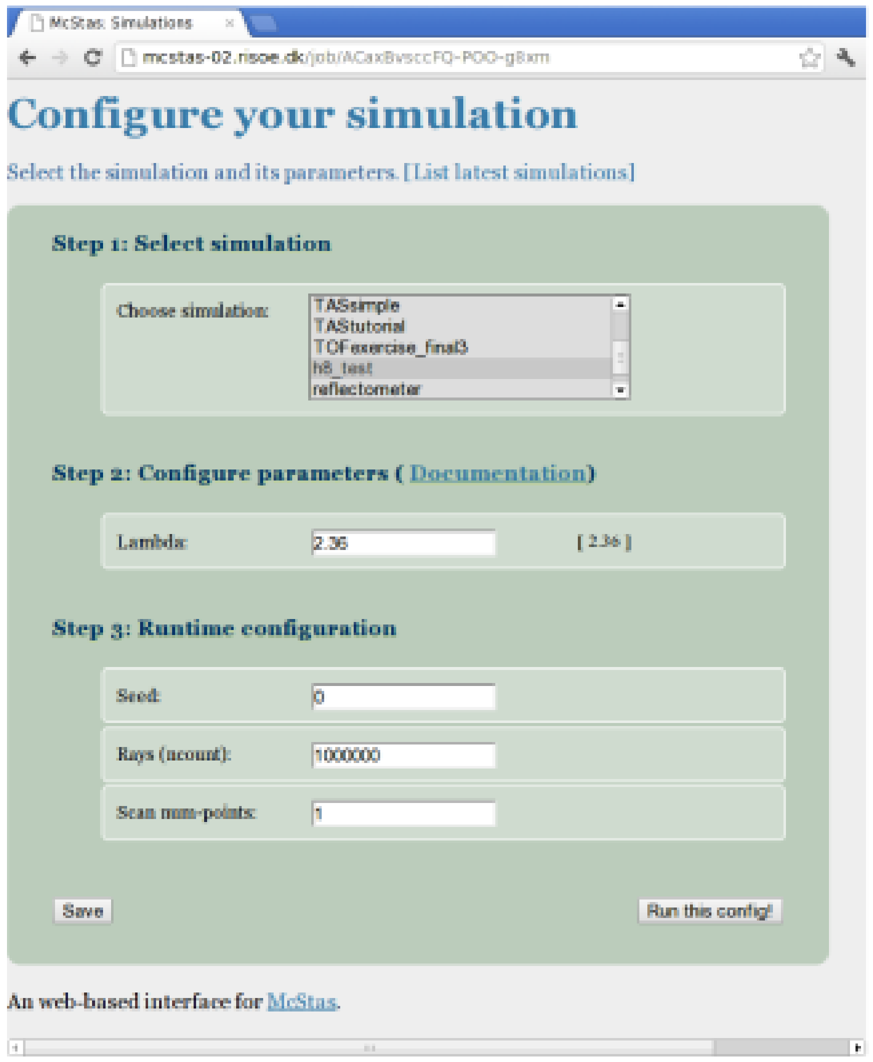
1. Configure

First, the instrument to simulate is chosen and configured. Parameters are adjusted and saved before the simulation is started.

2. Simulate

Once the simulation has been configured, it

Example: Configure



Configure your simulation

Select the simulation and its parameters. [List latest simulations]

Step 1: Select simulation

Choose simulation: TASsimple, TAStutorial, TOFexercise_final3, h8_test, reflectometer

Step 2: Configure parameters (Documentation)

Lambda: 2.36 [2.36]

Step 3: Runtime configuration

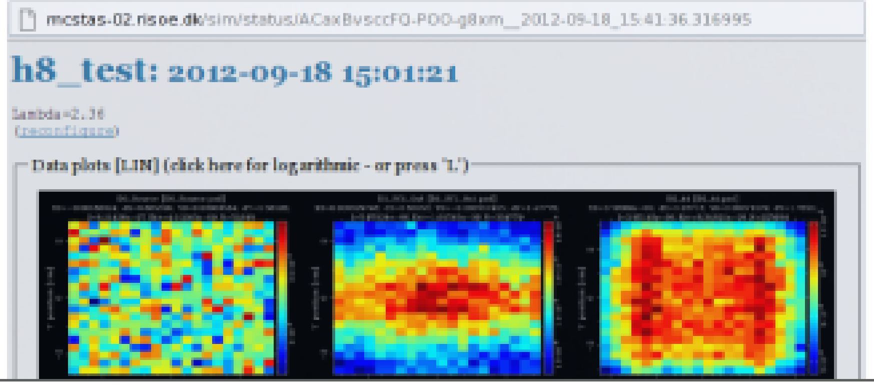
Seed: 0

Rays (ncount): 1000000

Scan num-points: 1

An web-based interface for McStas.

Example: Result overview


mcstas-02.risoe.dk/sim/status/ACaxBvsccFQ-POO-g8xm__2012-09-18_15:41:36.316995

h8_test: 2012-09-18 15:01:21

Lambda=2.36
(reconfigure)

Data plots [LIN] (click here for logarithmic - or press 'L')

Features

Permanent URLs: Both the URLs for configuration and results are unique and permanent; they can easily be shared with fellow students or colleagues.

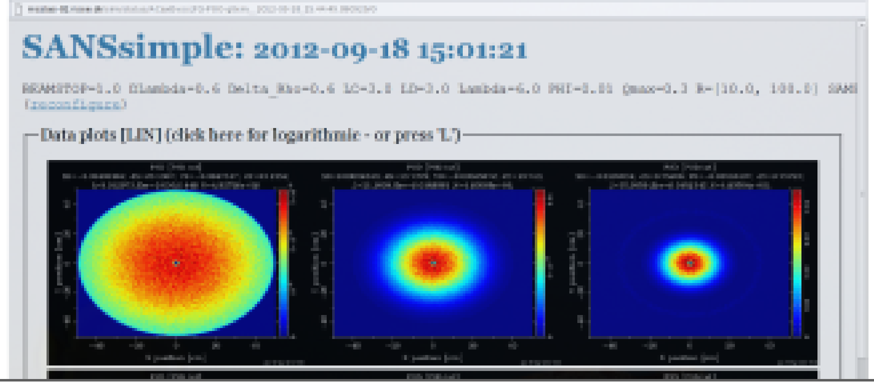
Parameter verification: A sanity check eliminates basic mistakes before running the simulation. Most helpful for students.

Authentication: A simple authentication measure prevents anonymous users from using the system.

Limits: Upper limits can be set for the neutron count to prevent users from running very long simulations.

Parallelism: Simulations can be run in parallel; both with many workers and on a per simulation basis using MPI.

Scanning a parameter



SANSsimple: 2012-09-18 15:01:21

BEAMSTOP=1.0 Dlambda=0.6 Delta_Rho=0.6 LC=3.0 LD=3.0 Lambda=6.0 PHI=0.01 Qmax=0.3 R=[10.0, 100.0] SANS
(reconfigure)

Data plots [LIN] (click here for logarithmic - or press 'L')

Other McStas 2.0 highlights

- Standardized parameter naming

- Updated library of the sources - common effort with Vitess
  - recommendation documents

- Split GUI/tool and calculation layer installations
  - mcstas-core, mcstas-comps, mcstas-tools-perl, mcstas-tools-python, ...

- Proper 64 support incl. MPI on Win64 and OS X

- New contributions in various areas

- Improved support for polarized neutrons
  - “All” components support polarized neutrons
  - Precession in tabulated magnetic fields

- Release in October 2012 (!!) - feel free to try the current dev tree
  - ~# svn co https://svn.mccode.org/svn/McCode
  - ~# ./configure --enable-mcstas

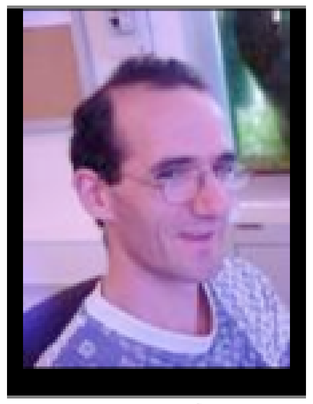
Conclusions incl. lessons learned

- McStas is a stable project and code
- Open Source strategy and modular design part of reasons for success
- Start out with healthy design
  - Original design by computer scientist, allowed physicists to expand like hell! Still rock solid! :-)
- Choose simple over complex or at least provide both options
- Flexibility is important - users are different
- Documentation is of key importance
- First user experience must be that “it works”
- Beyond 2.0 we will be applying “release often, release early...”

People

- The success of the project is also about the people:
  - Present McStas team members

- K Lefmann

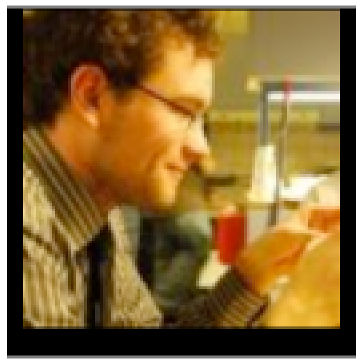


E Farhi

P Willendrup

E Knudsen

U Filges

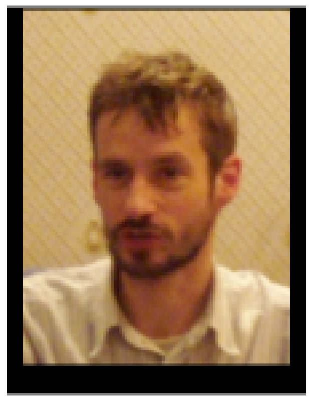


J Brinch

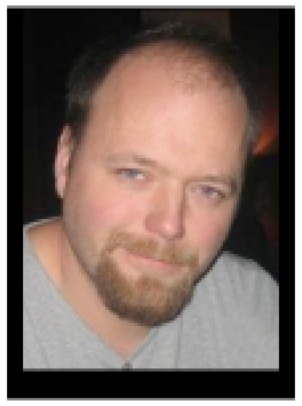
  - Past McStas team members

- K Nielsen

PO Åstrand



K Lieutenant



P Christiansen