



NOBUGS | 2016

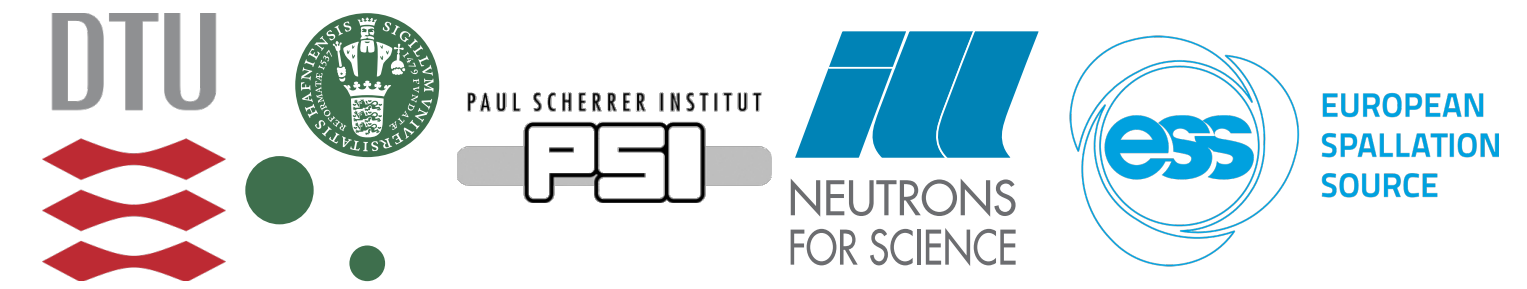
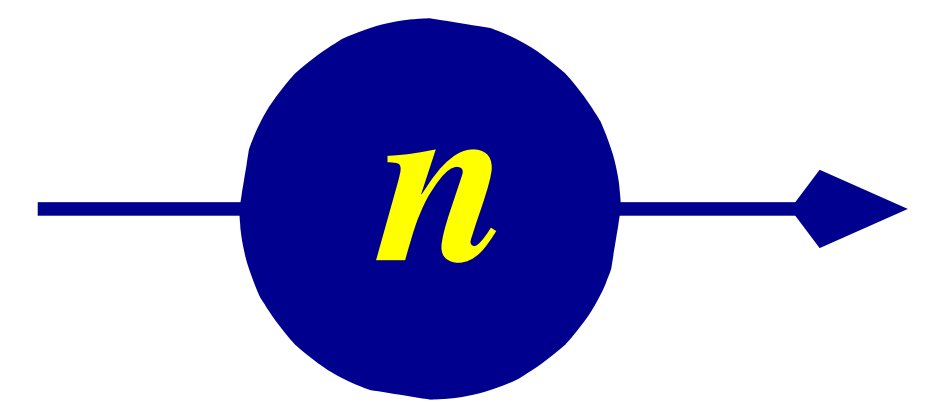
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NEW OPPORTUNITIES FOR BETTER USER GROUP SOFTWARE

New developments in the McStas neutron Monte Carlo ray-tracing package

P. Willendrup^{1,2}, E. B. Knudsen¹, E. Klinkby^{3,4}, T. R. Nielsen², J. Garde¹, E. Farhi⁵, M. Bertelsen⁶, T. Kittelmann⁴, K. Lefmann⁶

1. NEXMAP, Physics Department, Technical University of Denmark; pkwi@fysik.dtu.dk
2. ESS Data Management and Software Center, Copenhagen, Denmark
3. Center for Nuclear Technologies, Technical University of Denmark
4. European Spallation Source, Lund, Sweden
5. Institut Laue-Langevin, Grenoble, France
6. Niels Bohr Institute, Copenhagen, Denmark

McStas



ABSTRACT

The McStas neutron ray-tracing simulation package is a versatile tool for producing accurate simulations of neutron scattering instruments at reactors, short- and long-pulsed spallation sources such as the European Spallation Source. McStas It is extensively used for design and optimization of instruments, virtual experiments, data analysis and user training. McStas was founded as an scientific, open-source collaborative code in 1997.

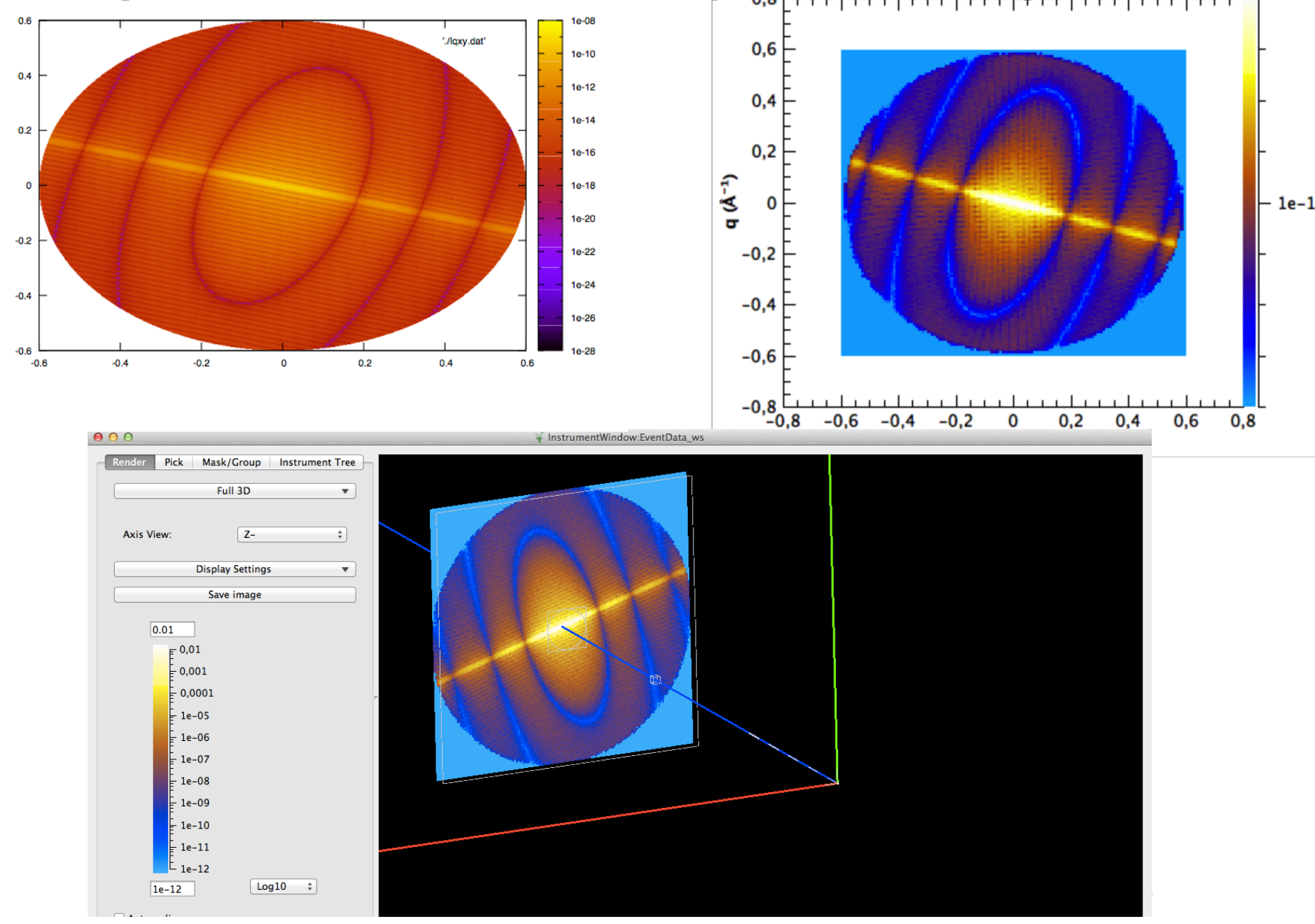
This contribution presents the project at its current state and gives an overview of lessons learned in areas of design process, development strategies, user contributions, quality assurance, documentation, interoperability and synergies with the McXtrace project.

Further, main new developments in McStas 2.3 (April 2016), McStas 2.4 (expected fall/winter 2016) and McStas 3.0 (expected 2017) are discussed, including many new components, updated source brilliance descriptions, new tools and user interfaces, web interfaces and a new interoperability with MCNP and other high-energy oriented Monte Carlo codes via the MCPL format.



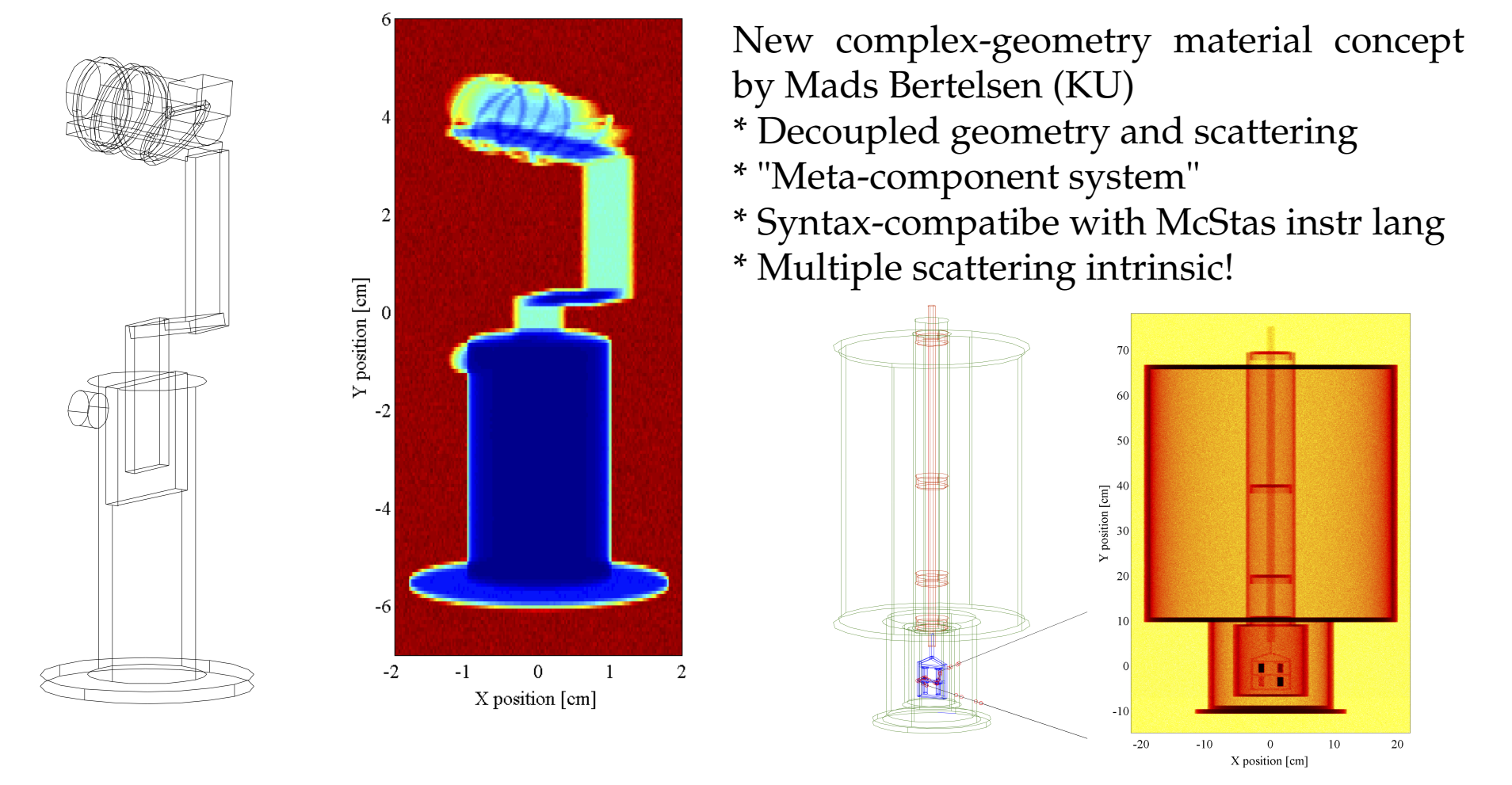
2.3: SASMODELS SAMPLE

SASview/SASmodels interface TR. Nielsen ESS Asymmetric scattering kernel "cylinders"



- Shown example is anisotropic "cylinders" kernel
- McStas 2.3 SasView_model.comp includes 58 functional kernels, see http://mcstas.org/download/components/samples/SasView_model.html

2.4: UNION CONCEPT



- New complex-geometry material concept by Mads Bertelsen (KU)
- * Decoupled geometry and scattering
- * "Meta-component system"
- * Syntax-compatible with McStas instr lang
- * Multiple scattering intrinsic!

INTRO

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) RSD
- Currently 2.5+1 people full time plus students

Project website at <http://www.mcstas.org> mcstas-users@mcstas.org mailinglist

What is McStas used for?

- Instrumentation
- Virtual experiments
- Data analysis
- Teaching (ILL, DTU)

Under-the-hood / inner workings

- Domain-specific language (DSL) based on compiler technology (LEX+YACC)
- Simple instrument language: C++ generation, ISO C
- Component codes realizing beamline parts (including user contribs)
- Library of common functions for e.g.
 - I/O
 - Random numbers
 - Physical constants
 - Propagation
 - Precision in fields

Open source - code available at <https://github.com/McStas/McXtrace/McCode>

2.3: CIF2HKL

cif2hkl webservice providing

- * Indirect McStas support for CIF
- * Easily Generate Single crystal an powder reflection list files
- * X-ray and neutron crosssections available *

Service available at <http://barns.ill.fr/cif2hkl.html>

FUTURE: NEW SAMPLES

Polycrystalline sample

A Cereser Phd work (DTU)

- * 1 st. Application "3DND", a tomographic diffraction-reconstruction technique, trace back near and far-field detector spots to a position in the sample

Simulated (powder) background from sample @ BL18 J-PARC

New samples in the pipe - SX + Phonons

PWillendrup with KU students

COMPONENTS, INSTRUMENTS

Neutron optics and other instrument components (we have ~150 comps)

Writing new comps or understanding existing is not that complex...

Check our long list of components and look inside... Most of them are quite simple and short... Statistics:

Example suite: ~100 instruments

Documentation

- Basic use info is available inside comp & instr codes, extracted by perl to html
- 100+ page manuals documenting
 - Metalinguage
 - What is "under the hood"
 - Examples of practical use plus advanced features
 - Algorithms and algorithms applied in the components
- More than 70 example instruments
- Various tutorial and teach yourself solutions are available

2.3: E-NEUTRONS.ORG

Free neutron e-learning platform with

- * Wiki-based textbook
- * Online quizzes and tests
- * Virtual experiments
- * Register at <https://www.e-neutrons.org>

FUTURE: 4D S(Q,W) VIA iFIT

S(Q, ω) via 'small displacements' from various sources:

PHON model (small displacements, <http://www.homepages.ucl.ac.uk/~ucfbdx/phon/>)
Quantum Espresso (DFT, <http://www.quantum-espresso.org>)
Atomistic Simulation Environment (simulation framework, <https://wiki.fysik.dtu.dk/ase/>)

2.3: MCPL PARTICLE FILES

MCPL info page

MCPL is short for Monte Carlo Particle List and is a particle interchange dataformat for Monte Carlo packages, written by Thomas Kittelmann, European Spallation Source.

MCPL will eventually include I/O wrappers for use with

- McStas and McXtrace - see also the [McCode Github page](https://github.com/McStas/McCode)
- MCNFS, MCNPX and MCNP6
- Geant4

- MCPL particle list format now supported - see <http://mcpl.mccode.org>
- Backends exist for McStas, McXtrace, Geant4 and MCNP/MCNPX is under development
- Recommended binary event list format for McStas

2.4: HIGHLIGHTS

- * Python mcdisplay-webgl-py
- * Complete Python tool suite by default
- * MCPL-based ESS_butterfly

MCSTAS SCHOOLS IN 2016

- * February 15th-19th, Bariloche, Argentina (CNEA)
- * May 30th-June 1st, Lund, Sweden (ESS only)
- * October 20th-21st, NOBUGS conference - see <https://indico.ess.lu.se/event/357/>

REFERENCES & FUNDING

1. Kim Lefmann, Kristian Nielsen. McStas, a General Software Package for Neutron Ray-tracing Simulations, Neutron News 10, 20, (1999).
2. Willendrup, P.; Knudsen E. B.; Klinkby E.; Farhi E.; Filges U.; Lefmann K; New developments in the McStas neutron instrument simulation package, J. Phys.: Conf. Ser. 528 012035 doi:10.1088/1742-6596/528/1/012035
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