New developments in the McStas neutron instrument simulation package

Willendrup, Peter Kjær; Bergbäck Knudsen, Erik; Klinkby, Esben Bryndt; R. Nielsen, Torben; Farhi, E.; Filges, U.; Lefmann, K.

Publication date:
2014

Citation (APA):
New developments in the McStas neutron instrument simulation package

Peter Willendrup\textsuperscript{1,2}, Erik Knudsen\textsuperscript{1}, Esben Klinkby\textsuperscript{3,4}, Torben R Nielsen\textsuperscript{2}, E Farhi\textsuperscript{5}, U Filges\textsuperscript{6}, K Lefmann\textsuperscript{7}

\textsuperscript{1}NEXMAP, Physics Department, Technical University of Denmark, Denmark
\textsuperscript{2}ESS Data Management & Software Center, Denmark
\textsuperscript{3}Center for Nuclear Technologies, Technical University of Denmark, Denmark
\textsuperscript{4}ESS Neutronics Group, Sweden
\textsuperscript{5}CS-group, Institut Laue-Langevin (ILL), France
\textsuperscript{6}LDM, Paul Scherrer Institute (PSI), Switzerland
\textsuperscript{7}eScience and Nano-Science centers, Niels Bohr Institute (NBI), Denmark
Agenda

- A brief introduction to McStas, Monte Carlo & raytracing
- Highlighted new features in McStas 2.1
  - McStas-MCNP for background estimates
  - McStas-Mantid event processing
  - Speedup in Single_crystal.comp
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, ESS.

- V. 1.0 by K Nielsen & K Lefmann (1998) RISØ.

- Currently 2.5+1 people full time plus students.

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

mcstas-users@mcstas.org mailinglist.
McXtrace - An X-ray ray-trace simulation package

McXtrace - Monte Carlo Xray Tracing, is a joint venture by

This site is undergoing reorganization, inconsistencies and broken links may occur. Please do report any findings to erkn_AT_ysik.dtu.dk if you have the time. Thanks in advance.

Funding from NABIT, DSF and the above parties.

McStas

New developments in McStas
McStas Introduction

World leading in neutron Monte Carlo

New developments in McStas
What is McStas used for?

- Instrumentation
- Virtual experiments
- Data analysis
- Teaching (KU, DTU)
Reliability - cross comparisons

- Much effort has gone into this
- Here: simulations vs. exp. at powder diffract. DMC, PSI
- The bottom line is
- McStas agrees 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 preparation

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.

McStas

Monochromatic neutron source

Detector

In Bragg scattering condition

Local, internal coordinate system!
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
McStas overview

• Portable code (Unix/Linux/Mac/Windoze)
  • Ran on everything from iPhone to 1000+ node cluster!

• 'Component' files (~150) inserted from library
  • Sources
  • Optics
  • Samples
  • Monitors
  • If needed, write your own comps

• DSL + ISO-C code gen.

New developments in McStas

Instrument file (average user, point/click, DSL)

Component (advanced user, modify from existing, c-code)

Kernel (McStas team)
Neutron optics and other instrument components

New developments in McStas
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:

Number of lines of code per component - 165 comps in total
Example suite: 123 instruments
New developments in McStas

1. Work on McStas-MCNPX interfaces for beam losses

Collaboration
- DTU Nutech
- DTU Fysik
- ESS

Mathematical expression:

\[ n_t = (r_t, v_t, t_t, s_t, p_i - p_r) \]

\[ n_r = (r_r, v_r, t_r, s_r, p_r) \]

Graphs showing dose vs. length along y [m] for neutrons and photons.
McStas-MCNPX interfaces for beam losses

\( n_t = (r_t, v_t, t_t, s_t, p_i - p_r) \)

\( n_i = (r_i, v_i, t_i, s_i, p_i) \)

\( n_r = (r_r, v_r, t_r, s_r, p_r) \)

Use: Check the Scatter_logger.comp in the McStas distribution

Future: Geant4, PHITS?

Collaboration:
- DTU Nutech
- DTU Fysik
- ESS

Journal of Physics: Conference Series Volume 528 conference I
McStas-Mantid event processing facilitated by:

- Special labels in component list
- Special Monitor_nD parameters
- IDF autogenerated by “mcdisplay” run
- NeXus output and LoadMcStas Mantid algorithm
McStas-Mantid event processing facilitated by:

- Special labels in component list
- Special Monitor_nD parameters
- IDF autogenerated by “mcdisplay” run
- NeXus output and LoadMcStas Mantid algorithm

Use: Check out templateSANS_Mantid from the McStas distribution - fully functional reduction
Events shown on the full instrument

- The event data from McStas should look something like this in "full 3D" - you may have to move/zoom a bit about
Events shown on the full instrument

- The event data from McStas should look something like this in "full 3D" - you may have to move/zoom a bit about

Use: Check out ILL_H16_IN5_Mantid from the McStas distribution - (not yet fully functional reduction)
Problem: McStas Single_crystal.comp “slow” for large unit cell diffraction studies

- Example: Rubredoxin

Rubredoxin

Images created from simulated datafile produced August 20th 2012 using 25 nodes on the DMSC cluster.

- Neutron count: 1e12
- Simulation time: \( \sim 10 + \sim 20 \text{ hr} = \sim 30 \text{ hrs total} \)

- Reflection list \( \sim 124 \text{ K reflections} \) (still “small” in the PX world!!)
Algorithm improvement: **Use incoming neutrons more efficiently** - scatter each one on all possible reflections

- **Red**: Original algorithm, one incoming neutron used only once
- **Blue**: Improved algorithm, each incoming neutron scattered (via SPLIT keyword) all possible times
- Component makes **estimate on average number of “active” diffraction spots** - in the case Rubredoxin this is around **50**!
Sim data speak for themselves - 1e9 rays

Old comp

New comp

~ Factor 50 more efficient

~ Factor 500 more efficient
Sim data speak for themselves - 1e9 rays

**Old comp**

```
[LOG] det [1e9_single/psd.dat]
X0=-7.56618; dX=97.4494; Y0=0.503148; dY=41.0417;
l=212.112 Err=1.14736 N=42254
```

Rubedoxin
124K reflections

```
[LOG] det [OldComp.BIG/1e9_single/psd.dat]
X0=-1.56177; dX=87.3014; Y0=0.292905; dY=37.9288;
l=297823 Err=0.554629 N=5950
```

**New comp**

```
[LOG] det [1e9_parallel/psd.dat]
X0=-6.35127; dX=97.5669; Y0=0.343201; dY=41.1348;
l=210.788 Err=0.162219 N=2.09642e+06
```

Predeuterated
1.7M reflections

```
[LOG] det [NewComp.BIG/1e9_parallel/psd.dat]
X0=-1.28883; dX=87.2793; Y0=0.16029; dY=37.366;
l=295512 Err=0.0207996 N=4.12822e+06
```

"~ Factor 50 more efficient"

"~ Factor 50 more efficient"

Use: Check out `template_NMX` from the McStas distribution

Similar optimisation of the PowderN component
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
  - T R Nielsen

• Past McStas team members

  - K Nielsen
  - PO Åstrand
  - K Lieutenant
  - P Christiansen
  - J Brinch

New developments in McStas