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.

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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

GNU GPL license
Open Source

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 erin_AT_fysik.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
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


New developments in McStas
Neutron ray/package:

- Weight (p): # neutrons in the package
- Coordinates (x,y,z)
- Velocity (v_x,v_y,v_z)
- Spin (s_x,s_y,s_z)

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

Local, internal coordinate system!

In Bragg scattering condition

McStas: key concepts

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

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McStas-MCNPX interfaces for beam losses

\[ \mathbf{n}_t = (r_t, v_t, t_t, s_t, p_i - p_r) \]

\[ \mathbf{n}_i = (r_i, v_i, t_i, s_i, p_i) \]

\[ \mathbf{n}_r = (r_r, v_r, t_r, s_r, p_r) \]

Collaboration
DTU Nutech
DTU Fysik
ESS
McStas-MCNPX interfaces for beam losses

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

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

Use: Check the Scatter_logger.comp in the McStas distribution

Future: Geant4, PHITS?

Journal of Physics: Conference Series Volume 528 conference 1
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
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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

1 timebin, 1000 x,y-bins

Rubredoxin

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

Neutron count: 1e12
Simulation time: \(~10 + \sim20\) hr = \sim30\) hrs total

- Reflection list \sim124\) K reflections (still “small” in the PX world!!)

Neutron count: 1e12
No gravitation
Xtal size: 0.5 mm
Xtal mosaicity: 12’
Detector: 50 x 50 cm flat
Detector-to-sample distance: 20 cm
Guide length: 131 m
Guide dimensions: 9.5 cm
\lambda_{min} = 1.3 \text{ Å}
\lambda_{max} = 3.5 \text{ Å}
Timespan: 51.39 to 143.4 ms
Divergence = 0.2 degs
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

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

New comp

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

~ Factor 50 more efficient

Rubedoxin
124K reflections

Predeuterated pyrophosphatase
1.7M reflections

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

Old comp

New comp

~ 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