New developments in the McStas neutron instrument simulation package

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New developments in the McStas neutron instrument simulation package

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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
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 (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.
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

1. Work on McStas-MCNPX interfaces for beam losses

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

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

Collaboration
DTU Nutech
DTU Fysik
ESS
New developments in McStas

- Work on McStas-MCNPX interfaces

Use: Check the Scatter_logger.comp in the McStas distribution

Future: Geant4, PHITS?

Collaboration:
- DTU Nutech
- DTU Fysik
- ESS

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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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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: ~10 + ~20 hr = ~30 hrs total

• Reflection list ~ 124 K reflections (still “small” in the PX world!!)

1 timebin, 1000 x,y-bins

Neutronecount: 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
$\lambda_{\text{min}} = 1.3 \ \text{Å}$
$\lambda_{\text{max}} = 3.5 \ \text{Å}$
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

New comp

~ Factor 50
more efficient

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

Old comp

Rubedoxin
124K reflections

New comp

Use: Check out template_NMX from the McStas distribution

Similar optimisation of the PowderN component

Old comp

New comp

~ Factor 50 more efficient

~ Factor 500 more efficient
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