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
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

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

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

- Work on McStas-MCNPX interfaces for beam losses

Mathematical expressions:

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

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

Collaboration:
- DTU Nutech
- DTU Fysik
- ESS
New developments in McStas

• MCNPX interfaces

Use: Check the Scatter_logger.comp in the McStas distribution

Future:

Geant4, PHITS?

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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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- 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 + ~20 hr = ~30 hrs total

- Reflection list ~ 124 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

New comp

Use: Check out template_NMX from the McStas distribution

~ Factor 50 more efficient

~ Factor 500 more efficient

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