Danish in-kind simulation efforts to the ESS - an overview

Klinkby, Esben Bryndt; Willendrup, Peter Kjær; Lefmann, Kim

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Esben Klinkby, DTU Nutech

contributions from:
Peter Willendrup (DTU)
Kim Lefmann (Uni Copenhagen)
Outline

- From hard protons to cold neutrons
  - Experimental overview
  - Simulation tools
  - "In house" simulation efforts
  - "In country" instrument design
Target station design

- Target station modeled with MCNPX
- Spallation takes place in rotating tungsten target
- The scale of the objects under study dictates the use of cold neutrons (~1-10meV)
- Neutrons are moderated in H\(_2\) and H\(_2\)O for cold and thermal neutrons
Flip-view

H2 moderator
Neutron guides

- Ni and Ti are chemically similar, but have very different refraction indices
- Coating with alternating layers: “Supermirrors” of which guides can be built which ~without loss, transport cold neutrons to radiation safe distances allowing ToF to be measured
Collimators & slits

- Works from the principle: Absorb anything which don’t have the desired direction (gadolinium)
- Discriminate beam in *space* and *divergence*
Disk Choppers

- Introduce pulses
- Discriminate beam in *time*
- Combining two choppers ~ Fermi chopper / velocity selector
Velocity selector

- Discriminate beam in *velocity / wavelength*
- $\Delta \lambda / \lambda \sim 10\%$
Fermi Choppers

- Discriminates beam in *time* and *wavelength* simultaneously
Crystal monochromators (and analyzers)

- Discriminate beam in *wavelength* by Bragg's law
- $\Delta \lambda / \lambda \sim 1\%$ (plus multiples $\lambda / 2$, $\lambda / 3$, ...)

![Image of crystal monochromator](image1)
![Image of crystal monochromator](image2)
Beamline design

- By a suitable selection of: choppers, velocity selectors etc etc the neutron scatterer is able to 'design' the beam optimal for his/her sample.
Some samples studied

- Numerous, cross-disciplinary
  - Materials in different states, eg.
    - Crystals
    - Powders
    - Molecules in solution
  - Material behaviour/function
    - Materials for fuel cells, batteries...
    - Magnets
    - Superconductors
    - Chemical reactions
    - Protein folding
    - Polymers
    - Metallurgy
    - ...
  - Å to m distances
  - Fourier (reciprocal space) methods
  - Direct space methods
Detectors

- Since neutrons are electrically neutral, they are difficult to detect.
- The preferred reaction is:
  \[ n + {^3\text{He}} \rightarrow {^3\text{H}} + p \]
due to the high cross-section
E field → protons collected → signal

- Recent years lack of \(^3\text{He}\) has forced the community to look for alternatives:
  \[ n + {^{10}\text{B}} \rightarrow {^7\text{Li}} + {^4\text{He}} \]
due to the high neutron capture cross-section of \(^{10}\text{B}\)
  The energetic nuclei ionize gas molecules which can be collected as signals
Monte Carlo techniques

- Los Alamos has since then developed and perfected many different monte carlo codes leading to what is today known as the codes MCNP5 and MCNPX.
- State of the art is MCNPX (or soon the merged MCNP6 code) that features numerous (even exotic) particles.
- MCNP was originally Monte Carlo Neutron Photon, later N-Particle.
- Mainly used for high-energy particle descriptions in weapons, power reactors and routinely used for estimating dose rates and needed shielding.
- Does not to date handle coherent scattering of neutrons due to the focus on high energies.
Ray-tracing methods

- When neutrons move in “free space”, we use ray-tracing - but in most cases in direction source → detector
- Of course parabolas rather than straight lines are used to implement gravity
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**: the code (of Risø origin) that encompass transport, beam-line and detector simulation, analysis framework
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.

Local, internal coordinate system!
What is McStas used for?

- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

KU, DTU 2005-2012
INSIS, NIDS, ESS workshops
Example from ILL

• Sources
• Optics
• Samples
• Monitors
• If needed, write your own comps
How to get from MCNPX to McStas

• Based on the latest MCNPX ESS target station (bi-spectral) geometry from ESS-Bilbao we have developed a McStas component mimicking both geometry and spectra.

• We are also working on alternatives which transport the neutron state directly, thus avoiding loss of phase-space / making assumptions.
Danish in-kind contributions

- 1.0 M€. Proton beam control (Søren Pape Møller, AU)
- 1.5 M€. Data Management and Software Center (Stig Skelboe, KU)
- 1.0 M€. Instrument simulation central office (Kim Lefmann KU, P. Willendrup DTU)
- 0.1 M€. Integrating moderator- and instrument simulations
  (B. Lauritzen, P. Willendrup, E. Nonbøl, E. Klinkby DTU)
- 0.2 M€. Radio-ecology baseline (Mikael Jensen, Sven Nielsen DTU)
- 0.1 M€. MANTID – DMSC (Stig Skelboe, KU)
- 0.8 M€. 5 DK-CH instrument packages
  (Niels Bech Christensen, DTU; Christian Rüegg, PSI)
Data Management and Software

• Staff: Stig Skelboe, Thomas Rod, Lars Melvyn, (secretary) (3 FTE)
• Supporters: scientists from KU, DTU-Risø, AU

• DMSC scope (under planning)
  – User service
  – Instrument control
  – Data acquisition
  – Data archiving
  – Data visualization and analysis
  – (science modeling)
  – Instrument simulation
Instrument simulations

• Simulate a suite of simple instruments to investigate time structure
  – Later: move towards detailed instrument descriptions
• Answer questions from ESS instrument responsibles
  – Compare thermal powder diffraction designs
  – Compare thermal spectrometer designs
  – Analyze effect of off-specular scattering
• Prepare for virtual experiments for data analysis
  – Event mode data; bootstrap
  – Effect of the pulse tail
  – Effect of multiple scattering; sample environment
• Maintain and develop McStas
• Study guide systems
  – Long thermal guides
  – Guide bundles
  – Bi-spectral extraction
• Support function for simulators
Example: Cold chopper spectrometer

- 100 m elliptical guide
- Wavelength multiplication at sample
- 30 (300) times IN5 flux
- Count rates of the order $10^8 / \text{sec.}$
- VE shows expected resolution
- Moderator “Hot spot” is highly beneficial
Conclusions

• Danish universities are/will be heavy involved in many aspects of the design, construction and usage of the ESS and its instruments, including:

→ Data management
→ Radioecology
→ Instrument simulation
→ Instrument design
→ Neutron scattering experiments
→ Neutronics
→ Develop/maintain McStas
Backup slides...
Overview
Moderators... (Where McStas starts)

\[ I(x,y,E,t) \text{ from neutronics} \]

\[ \Omega_{BL}(x,y) \]

\[ \text{Per beamline:} \quad I_{BL}(x,y,E,t) = \frac{\Omega_{BL}(x,y)}{4\pi} I(x,y,E,t) \]
Example suite: 7 TOF spectrometers:

- ESS_IN5_reprate.instr
- ILL_BRISP.instr (Small-angle)
- ILL_H15_IN6.instr
- ILL_H16_IN5.instr
- ISIS_Hetfull.instr
- PSI_Focus.instr
- templateTOF.instr
Example suite: 5 TAS

• ILL_H142_IN12.instr
• ILL_H25_IN22.instr
• h8_test.instr
• templateTAS.instr
• linup-1.instr (Risø TAS 1)
• linup-2.instr
• linup-3.instr
• linup-4.instr
• linup-5.instr
• linup-6.instr
• linup-7.instr
Example suite: 1 Hybrid spectrometer + 1 Spin-echo
Example suite: Large scale structures
Example suite: Diffractometers

- ILL_D1A.instr
- PSI_DMC.instr
- templateDIFF.instr
- templateLaue.instr
Example suite: Imaging