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

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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\textsubscript{2} and H\textsubscript{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 $\lambda/2$, $\lambda/3$, $\ldots$)
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 $\rightarrow$ protons collected $\rightarrow$ 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 \( (p) \): Number of 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.
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 $10^8$ / 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)

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

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

Per beamline:
\[ I_{BL}(x,y,E,t) = \frac{\Omega_{BL}(x,y)}{4\pi} I(x,y,E,t) \]
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