Simulating neutrons ::

Moderation, extraction, shielding

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www.europeanspallationsource.se
CONTENTS

- Cradle to grave:
  - Spallation
  - Moderation
  - Extraction
  - Backgrounds & Shielding
- Software interfaces
- Possible configurations
TDR configuration :: 2 tall moderators

- Neutrons extracted through window at 2m
- Instrument separation: 5° (=> 17.5 cm at 2m)
- Guides should bend to avoid streaming of fast neutrons
Neutron creation:: spallation

- Proton de Broglie wavelength:
  \[ \lambda = \frac{hc}{(2m_p c^2 E_p)^{\frac{1}{2}}} = 6 \cdot 10^{-16} \text{ m} \]

  Size of nuclei: \( \sim 10^{-14} \text{ m} \)

- \( \Rightarrow \) protons interact with nucleons not nuclei
- Spallation is efficient: \( \sim 70 \) neutrons pr proton at 2GeV
- Theoretically complicated: software use models

Alternatively: use reactors: Continuous source
Neutron moderation :: from MeV to meV

• Scattering instruments probe distances: 
  \( \sim \AA = 10^{-10} \text{ m} \Rightarrow \text{neutrons must be cooled to meV.} \)

• \( n, H \) cross-section is large \( \rightarrow \) Water is efficient for thermalization. A few cm is sufficient

• 20K Para-hydrogen (spin flip scattering) is used. 
  \( \sim 1 \text{ cm} \) is sufficient

• Para-hydrogen \( \sim \) transparent for cold neutrons

• Simulation wise, the interactions of protons with the target, neutron creation and moderation is modeled using \( MCNP \)
MCNPX :: Monte Carlo N-Particle Transport Code

- Standard MC code for neutron physics (spallation sources, reactors, weapons...)
- Use Evaluated Nuclear Data – ENDF-VII
- Use INCL, Bertini, Isabel or CEM
- Limitations:
  → Most applications based on free gas model. Coherent scattering only accurate for powders.
  → Must be supplemented with scattering kernels for accurate description of processes at low energy (eV range)
  → Slow
  → Licensing: distribution is restricted, personal license required

History box

- During WW2, “numerical experiments” were applied at Los Alamos for solving mathematical complications of computing fission, criticality, neutronics, hydrodynamics, thermonuclear detonation etc.
- Notable fathers: Neuman, Ulam Metropolis
- Named “Monte Carlo” after Ulam’s fathers frequent visits to the Monte Carlo casino in Las Vegas
- Initially “implemented” by letting large numbers of women use tabularized random numbers and hand calculators for individual particle calculations
- Later, analogue and digital computing devices were used
Ray tracing techniques

- Instrument Monte Carlo methods implement coherent scattering effects.
- Uses deterministic propagation whenever possible.
- 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.

Numerous codes exist:

- NISP
- IDEAS
- Instrument Builder
- McVine
- RESTRAX/SIMRES
- VITESS
- McStas,
- NADS
- PHITS
- NTRANS

- Result: A realistic and CPU-time efficient transport of neutrons in the thermal and cold range.
Getting neutrons from A to B

- \( \text{Ni} \) and \( \text{Ti} \): chemically similar, but different refraction indices

\[ q = 2k \sin(\theta) \]

\[ \theta \]

\[ k_i \]

\[ k_f \]

⇒ Coating with alternating layers: “Supermirrors”
⇒ Neutron guides
⇒ Transport cold/thermal neutrons (~without loss) to radiation safe distances
⇒ Energy measurement by TimeOfFlight.

All of this + choppers, velocity selectors, collimators, monocrometers etc is simulated in eg McStas
Instrument optimizations :: cold source

- Important to take into account non-uniformities.
- Source is parametrized in *McStas* using below (*MCNP*) distributions.

![Graph showing average cold brightness vs vertical position for different distances.](image1)

![Graph showing average cold brightness vs horizontal position for different distances.](image2)

![Illustration of moderator image with reflector and target sides.](image3)
Instrument optimizations :: thermal source

- Important to take into account non-uniformities.
- Source is parametrized in *McStas* using below (*MCNP*) distributions.
Phase-space for instrument optimization is huge

To ease the task, one additional layer of software is added on top of McStas: *guide_bot*

Given a user-selected set of *components* and allowed *parameters*, *dimensions* etc, *guide_bot* uses a Swarm algorithm to find the guide which best transfer the beam from the beam extraction to the sample

Example: elliptical-elliptical, ...

**Example of guide_bot output**

- Vertical cut
- Horizontal cut
- Horizontal divergence
- Vert. div.
- 100% trans.

$\lambda = 2\text{Å}, 6\text{Å}$
Shielding and backgrounds

- In addition to cold/thermal neutrons, sample and detectors are subject to backgrounds (n, π, γ, p, from the spallation hotspot + secondaries).
- Not naturally incorporated in ray-tracing codes
- Ongoing efforts to mirror the MCNP model of target, moderators, reflectors and beam extraction in GEANT4 (used for detector simulations).
Shielding and backgrounds :: Fast neutrons

Reflector material choice, impacts shielding requirements

\( \text{n/cm}^2/\text{primary proton} \) 
\( E > 0.1 \text{ MeV} \)
Shielding and backgrounds

- To estimate shielding and background, individual neutron states are handed from \textit{MCNP} to a \textit{ROOT} based analysis framework.
- Avoids inaccuracies from integration
Monte Carlo vs. ray tracing – where are we heading?

- MCNP: target, moderator, reflector design
- McStas (+guide_bot) for instrument design
- GEANT4 for shielding and backgrounds
- Vitess & NADS & Particle swarms: shielding & optics
  - design documentation for the instrument
- MCNP: safety, dose-rates (future use of FLUKA or MARS)
- GEANT4: detector design

⇒ Interfacing is important.
- Efforts ongoing to merge and benchmark
Example :: MCNP-McStas interface

I. Neutrons generated with MCNPX
II. Handed to McStas through SSW interface
III. Unreflected neutrons returned to MCNPX for dose-rate calculation
Example :: MCNP-McStas interface

I. Neutrons generated with MCNPX
II. Handed to McStas through SSW interface
III. Unreflected neutrons returned to MCNPX for dose-rate calculation
The moderator design at ESS is close to completion. Recommendations from instruments:
- One flat ~3cm moderator above target +
- One taller ~6cm x 6cm below target

Some options for lower moderator are:

- TDR like cylinder
- Tube moderator

Final decision by October this year
Example of $D_2$ moderator – not optimized

<table>
<thead>
<tr>
<th>Case</th>
<th>Volume $D_2$ moderator (below)</th>
<th>Flat $H_2$ moderator (above)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference</td>
<td>$6.83 \times 10^{12}$</td>
<td>$3.34 \times 10^{13}$</td>
</tr>
<tr>
<td>1a</td>
<td>$4.56 \times 10^{12}$</td>
<td>$2.80 \times 10^{13}$</td>
</tr>
<tr>
<td>1b</td>
<td>$2.85 \times 10^{15}$</td>
<td>$3.22 \times 10^{13}$</td>
</tr>
</tbody>
</table>

From arXiv:1401.6003
ESS moderator team

- Neutronics Group
  - K. Batkov, E. Klinkby, T. Schönfeldt, A. Takibayev, L. Zanini
- Plus
  - F. Mezei, G. Muhrer, E. Pitcher

Thanks to Phil Bentley for input
Ask me!

Or visit eg:

http://mcstas.org/

https://svn.mccode.org/svn/GuideBot

Example: Background along guide

I. Neutrons generated with MCNPX  
II. Handed to McStas through SSW interface [1]  
III. Unreflected neutrons returned to MCNPX for dose-rate calculation

Guide end overilluminated by energetic neutrons

![Guide cross-section diagram]
Example: Background along guide

- **Straight guide**

- **Curved guide (r_{curvature} = 1500m)**

Dose-rates, measured 5cm in the steel converted from flux according to official Swedish radiation protection procedures

- Line-of-sight lost
Example: Background along guide

- Restricting to $\lambda \in \{0.5 \text{ Å} - 1.0 \text{ Å}\}$
- Photon dose-rate follows neutron dose-rate ✓
Scales are off by about 50% (comparing 1a to 1b) → poor man's rescale