Simulating neutrons - Moderation, extraction, shielding

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Publication date: 2014

Citation (APA):
Simulating neutrons ::
Moderation, extraction, shielding

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nēn at ESS - CERN, June 12-13, 2014

www.europeanspallationsource.se
CONTENTS

- Cradle to grave:
  - Spallation
  - Moderation
  - Extraction
  - Backgrounds & Shielding
- Software interfaces
- Possible configurations
- 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:
  \[ \lambda = \frac{h c}{(2m_p c^2 E_p)^{\frac{1}{2}}} = 6 \cdot 10^{-16} \text{ m} \]

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: 
  \( \sim \text{Å} = 10^{-10} \text{ m} \Rightarrow \text{neutrons most be cooled to meV.} \)

• \( n, H \) 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 \( \text{MCNP} \)
• 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

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

\[ \Rightarrow \text{Coating with alternating layers: “Supermirrors”} \]

\[ \Rightarrow \text{Neutron guides} \]

\[ \Rightarrow \text{Transport cold/thermal neutrons (~without loss) to radiation safe distances} \]

\[ \Rightarrow \text{Energy measurement by TimeOfFlight.} \]

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.
Instrument optimizations :: thermal source

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

- 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*

![Diagram showing phase-space cuts for guide_bot output with parameters: \( \lambda = 2\,\text{Å}, 6\,\text{Å} \)]
In addition to cold/thermal neutrons, sample and detectors are subject to backgrounds ($n, \pi, \gamma, p$, 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

$n/cm^2/primary\ proton\ \ E>0.1\ MeV$
Shielding and backgrounds

To estimate shielding and background, individual neutron states are handed from MCNP to a ROOT based analysis framework.

Avoids inaccuracies from integration.

Neutron spectrum at beam extraction (radii=2m)
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
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>3.34x10$^{13}$</td>
<td>6.83x10$^{12}$</td>
</tr>
<tr>
<td>1a</td>
<td>2.80x10$^{13}$</td>
<td>4.56x10$^{12}$</td>
</tr>
<tr>
<td>1b</td>
<td>3.22x10$^{13}$</td>
<td>4.56x10$^{12}$</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
Backup slides
Learn more

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 cross-section

Guide end overilluminated by energetic neutrons
Example: Background along guide

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

- Restricting to $\lambda \in \{0.5 \AA - 1.0 \AA\}$
- Photon dose-rate follows neutron dose-rate ✓
Deuterium spectra

Scales are off by about 50% (comparing 1a to 1b) → poor man's rescale