Simulating neutrons - Moderation, extraction, shielding

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

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 → 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 \textit{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

- \textit{Ni} and \textit{Ti}: chemically similar, but different refraction indices

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

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

All of this +\textit{choppers}, \textit{velocity selectors}, \textit{collimators}, \textit{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.
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
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

n/cm²/primary proton
\[ E > 0.1 \text{ MeV} \]
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
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
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II. Handed to McStas through SSW interface
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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

Viewed from the side
More bright than cylinder, but also more directional, and can serve less instr.

Viewed from the side
Unlikely given the recommendations, but still not excluded. Interesting for nnbar
Example of $D_2$ moderator – not optimized

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
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 of guide cross-section with 2cm and 50cm dimensions]

![Graph of Log(intensity) vs. \( \lambda [\text{Å}] \)]

![Heatmap of neutron channel and steel regions]
Example: Background along guide

- 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

- Straight guide
- Curved guide ($r_{\text{curvature}} = 1500\text{m}$)

- Photon dose-rate follows neutron dose-rate

- Restricting to $\lambda \in \{0.5 \text{ Å} – 1.0 \text{ Å}\}$

- Line-of-sight lost

- Photon dose-rate follows neutron dose-rate $\checkmark$
Deuterium spectra

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