Simulating neutrons - Moderation, extraction, shielding

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Simulating neutrons ::
Moderation, extraction, shielding

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

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

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

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

- Scattering instruments probe distances: 
  \[\sim \text{Å} = 10^{-10} \text{ m} \Rightarrow \text{neutrons must be cooled to meV.}\]

- 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

<table>
<thead>
<tr>
<th>Numerous codes exist:</th>
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<tbody>
<tr>
<td>NISP</td>
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<tr>
<td>IDEAS</td>
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<td>Instrument Builder</td>
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<td>McVine</td>
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<td>RESTRAX/SIMRES</td>
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<td>VITESS</td>
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<td>McStas,</td>
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<td>NTRANS</td>
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- 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

⇒ 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, velocity selectors, collimators, monocrometers etc} is simulated in eg \textit{McStas}
Instrument optimizations :: cold source

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

![Graphs showing average cold brightness vs. vertical and horizontal positions.](image-url)
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 transfers the beam from the beam extraction to the sample
- Example: elliptical-elliptical, ...

**Example of `guide_bot` output**

- Vertical cut
- Horizontal cut
- Horizontal divergence
- \( \lambda = 2\text{Å}, 6\text{Å} \)
- 100% trans.
Shielding and backgrounds

- 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/cm²/primary proton $E>0.1$ MeV
To estimate shielding and background, individual neutron states are handed from MCNP to a 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
Design status

- 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
  - Lower moderator, viewed from above

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

- Final decision by October this year

- Viewed from the side
  - Unlikely given the recommendations, but still not excluded. Interesting for nnbar
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>
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</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>$4.56 \times 10^{12}$</td>
<td>$3.22 \times 10^{13}$</td>
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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

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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
Example: Background along guide

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

- 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 (radius of curvature $r_{\text{curvature}} = 1500 \text{m}$)

- Restricting to $\lambda \in \{0.5 \, \text{Å} - 1.0 \, \text{Å}\}$
- Photon dose-rate follows neutron dose-rate \( \checkmark \)
Deuterium spectra

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