Tools envisaged to address questions, short term and long term goals

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Tools envisaged to address questions, short term and long term goals

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www.europeanspallationsource.se
“Conventional” simulations at ESS
- Spallation/Moderation/Extraction
- Backgrounds & Shielding
- Ray-tracing
- Detectors

Present approach to \( nn\bar{n} \) simulations at ESS

Future integration of \( nn\bar{n} \) efforts to ESS coding framework
Step 1 :: Neutron creation & moderation

Starting point = First interface:
Proton source at -1.5m following spatial and angular distributions based on accelerator simulations.
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=MCNPX, 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 → 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 \( \text{MCNP} \), heavily dependent on scattering kernels
Neutrons extracted through window at 2m
Instrument separation: $5^\circ$ ($\Rightarrow$ 17.5 cm at 2m)
NNbar port concept

Preliminary engineering concept from R. Linander
NNbar port concept

Preliminary engineering concept from R. Linander

Need to be followed by changes to the TMR plug (cutout of Be+S.S.)
NNbar port concept

Preliminary engineering concept from R. Linander

Extraction port converted to neutron scattering beamlines after nnbar is decommissioned
Step 2 :: 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

Result: A realistic and CPU-time efficient transport of neutrons in the thermal and cold range
- Essential that the limitations are treated seriously and that the input is accurate

Numerous codes exist:
- NISP
- IDEAS
- Instrument Builder
- McVine
- RESTRAX/SIMRES
- VITESS
- McStas,
- NADS
- PHITS
- NTRANS
Correlations and non-uniformity is handled by transferring individual events from one code to the next, or by carefully fitting the full parameter space, taking into account significant correlations.

Software written to transfer events to ROOT, McStas. GEANT4 is upcoming.
Instrument optimizations :: cold source

- Source is parametrized in *McStas* using below (*MCNP*) distributions
- Revisited as soon as moderator decision is final

![Graphs showing average cold brightness vs. vertical and horizontal positions](image)
Getting lowE neutrons from A to B

- Ni and 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 +choppers, velocity selectors, collimators, monocrometers etc is simulated in eg McStas

Also effects of gravity and magnetic field, can be included into the McStas simulation
Instrument optimizations :: guide_bot

- 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, …

- Once a McStas version of the nnbar instrument exists, guide_bot could aid optimizing
Step 3 :: 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).
To estimate shielding and background, individual neutron states are handed from MCNP to a ROOT based analysis framework. Avoids inaccuracies from integration.
ESS Detector Group developed a framework for simulations neutron facility phenomena, used also by Shielding and Optics group.

- Based on GEANT4, adding extensions relevant for a neutron facility (crystal diffraction, thermal scattering, ...)
- Flexible to any input generator, collaboration with Target for full integration (MCNP → GEANT4)

**Neutron diffraction in polycrystals (Al, Cu, ...)**

- Neutrons with $\lambda \approx 1$ Å scatters coherently on crystal planes at angles given by Bragg condition:
  $$2d \sin \theta = n \lambda$$
- Affects X-section and angular distribution:
- [Image of neutron diffraction diagram]

- NXSLib by M. Boin provides first principle calculation of relevant quantities, based on crystal unit cell definition:
  - [Image of NXSLib diagram]
  - Unit cell must be associated to G4Material during geometry construction
  - Details of Geant4/NXSLib integration to be described in separate paper
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
Fitting $nn$ simulations into framework:

- **MCNPX**
  - Particle List
  - Distributions
  - E. Klinkby. / ESS
  - L. Castellanos /UT

- **NTRANS**
- **MCSTAS**
  - Y. Kamyshkov, M. Frost /UT
  - C. Theroine /ESS, M. Frost /UT

- Magnetic field w.
- Active/passive shield
- Simulation or measurements

- Residual pressure input

- n – crossing with annihilation target

Neutron tracing in n-nbar setup with gravity, Super Mirror Reflections, lay-out and parameter optimization, timing.
Provide: sensitivity, distributions, particle lists, shielding input; backgrounds of gammas, p, fast n, muons
Fitting $nn$ simulations into framework: annihilation & detectors

Detector configuration

Backgrounds:
• Fast neutrons, beam
• Cosmic
• $(n, \gamma)$

Optimization goals:
• High $n\bar{n}$ detection efficiency
• Background suppression

GEANT4

INR $NN\bar{n}$ generator

GENIE $\nu$ generator

E. Golubeva / INR

R. Pattie / NCSU/LANL

D. Phillips / NCSU

Performance/optimization studies
• From CINTER: Nitrogen 19 is the main contributor of delayed neutrons (> 90%).

• The production rate in the tungsten target wheel is ~0.03 neutrons/cm³/s (at 5MW) after 0 seconds (average over the whole wheel 170E3 cm³).

• To get a feeling for how this compares to the total neutron production:
  • ~40 neutrons per proton => 6E17 neutrons/s

• I'll bet a beer that fast neutrons (and other fast) that scatter/partially moderate somewhere close to the detector is a bigger problem than delayed neutrons from the target
Conclusions & Future work

- **McStas** simulations is being benchmarked against **NTRANS** *(see Matt's talk)*
  
  I. Lacking: final moderator decision + (positive) decision of beam extraction + assess impact on TMR plug

  II. → new **MCNP** input / events file (Esben)

  III. Will need simulation of magnetic field impact on each individual neutron trajectory (need a dummy map and some software development in McStas / NTRANS). *(who? Input from Gustaaf/Yuri)*

- **Genie/INR** coupling to the ESS detector framework *(GEANT4)*,

  I. Eventually to ease the simulation of realistic backgrounds (e.g. from **MCNP** event files) *(who? David?, Esben?)*

Note: ESS as well as it's software is being developed on the fly, nn will have to cope

- **MCNP** is working from inside-out and **GEANT4** is working from outside-in, both based on ENDF-VII cross-section data.

- Having more codes with overlap is very useful for debugging purposes

- Interfaces are necessary but should be used with caution (avoid integration)
Major contributors

- Y. Kamyshkov
- T. Kittelmann (ESS Detectors)
- P. Bentley (ESS Optics & shielding)
- R. Linander K. Batkov, T. Schönfeldt, A. Takibayev, L. Zanini (ESS Target)
Backup slides
Instrument optimizations :: thermal source

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

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**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
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
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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:
  - 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 exclude 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>
</tr>
</thead>
<tbody>
<tr>
<td>Reference</td>
<td></td>
<td>3.34 x 10^{13}</td>
</tr>
<tr>
<td>1a</td>
<td>6.83 x 10^{12}</td>
<td>2.80 x 10^{13}</td>
</tr>
<tr>
<td>1b</td>
<td>4.56 x 10^{12}</td>
<td>3.22 x 10^{13}</td>
</tr>
</tbody>
</table>

- From arXiv:1401.6003

TDR

1a
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

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**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
Deuterium spectra

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