Simulation and experimental validation of advanced neutron moderators

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CRP: Advanced moderators for intense cold neutron beams in materials research; Simulation and experimental validation of advanced neutron moderators

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Outline

• Simulation with McStas & MCNPX
• DTU contribution to CRP
  – Directional high brightness moderators
  – Towards cold moderators using high albedo materials
DTU's contribution to the CRP

A. Description of Research Objectives and anticipated outcomes
Expand MCNPX-McStas interface to properly describe new high-albedo materials anticipated for advanced moderator concepts

B. Scientific Scope
Assess the performance of new materials and geometries proposed for advanced moderators through simulations and experiments. One of these novel materials is nano-diamonds
DTU's contribution to the CRP

C. Year 1
Participate in flat moderator experiments (ESS initiated).
Develop the computational tools, for simulation of high-albedo materials

D. Year 2
Build and test a prototype of an advanced moderator based on high-albedo materials (with ESS) → validation of the simulation codes

E. Year 3
Finalize code, based on lessons from years 1 & 2
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Directional enhancement from geometrical considerations

Thermal neutrons

Peaks close to cold vessel walls moves closer as the height decrease ⇒ increased brightness (but decreased flux)

Note: Made possible from SSW→ROOT interface
Directional enhancement from geometrical considerations

Para-hydrogen cross-section
⇒ most thermal neutrons cooled within ~1cm
⇒ emitted “freely”
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Nano diamonds – experimental mock-up

Para-hydrogen

Nano-diamond reflectivity

Nano diamonds – experimental mock-up

Quasi-elastic scattering

Incoming fast neutron

Nano-diamond reflectivity

Para-hydrogen cross section

Outgoing cold neutron
Nano-diamonds purchased
Summery

- Directional moderator developed at ESS
- Experimental validation being planned
- MCNPX-McStas coupling well established
  - But yet no attempts made to introduce high-albedo materials
- Nano-diamonds purchased, characterization experiments is being planned
Backup
Elements of Monte-Carlo ray-tracing - McStas

- Instrument simulation using Monte Carlo ray-tracing methods implement coherent scattering effects
- Uses deterministic propagation where this can be done
- 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 efficient transport of neutrons in the thermal and cold range, i.e. below 0.025 eV.
Neutron ray/package:
- Weight (p): # neutrons (left) in the package
- Coordinates (x, y, z)
- Velocity (v_x, v_y, v_z)
- Spin (s_x, s_y, s_z)

Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.

Key concepts:
- Time (t)
- Monochromatic neutron source
- Bragg scattering condition
- Local, internal coordinate system!

Components: Here the neutron physics happen, neutron weight adjusted according to scattering probabilities etc.
Interfaces to other codes important

- Interface-code coupling McStas and MCNP
- Interoperability with Vitess (mcstas2vitess)
- Interoperability with various other codes via files (Tripoli4, GeomView, Crystallographica)
The task:

“Interfacing the MCNP and McStas Monte Carlo codes for improved optimization of the ESS moderator-beam extraction systems”

The solutions:

- Tally
- Ptrac
- SSW
- Supermirror
- Compile
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The solutions:

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- Compile
SSW MCNPX-McStas coupling – example of use for background calculations

At each scattering, for any McStas component (e.g., a guide), the incoming and outgoing neutron state can be temporally stored & analyzed.

**At each scattering:**

- **Incomming state:** \( \mathbf{n}_{\text{in}} = (\mathbf{x}_{\text{in}}, \mathbf{v}_{\text{in}}, t, w_{\text{in}}) \)
- **Transmitted state:** \( \mathbf{n}_{\text{trans}} = (\mathbf{x}_{\text{in}}, \mathbf{v}_{\text{in}}, t, w_{\text{trans}}) \)
- **Reflected state:** \( \mathbf{n}_{\text{refl}} = (\mathbf{x}_{\text{out}}, \mathbf{v}_{\text{in}^{-}}, t, w_{\text{in}^{-}} - w_{\text{trans}}) \)

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Source/origin

Neutron trace

Guide wall

Detector
Background along guide

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

Guide end over-illuminated by energetic neutrons

![Guide cross-section](image)

![Graph showing neutron channel](image)
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)
Example: Background along guide

Straight guide

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

- Restricting to $\lambda \in \{0.5 \ \text{Å} - 1.0 \ \text{Å}\}$
- Photon dose-rate follows neutron dose-rate

Line-of-sight lost