MCNPX-McStas interface for cold/thermal neutron moderator and guide simulation

Klinkby, Esben Bryndt; Lauritzen, Bent; Nonbøl, Erik; Willendrup, Peter Kjær; Filges, Uwe; Panzner, Tobias

Publication date: 2012

Citation (APA):

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.
MCNPX-McStas interface for cold/thermal neutron moderator and guide simulation

Esben Klinkby
Bent Lauritzen
Erik Nonbøl
Peter Willendrup
Uwe Filges (PSI)
Tobias Panzner (PSI)
Motivation

- Traditionally two decoupled Monte Carlo codes cover different needs in Neutron Scattering simulations:
  - MCNP/X used for TMS calculations
  - Neutron ray tracing code, e.g. McStas (talks by P. Willendrup & E. Farhi) used for instrument design + data analysis

- Even more precise simulations may be possible by combining the best of the two worlds: The detailed description of incoherent scattering from MCNP/X with the coherent scattering of McStas.

- **Prospects**: usage of direct MCNP/X McStas coupling:
  - Optimization of complex moderator design
  - Shielding calculations along neutron guide
  - Crosstalk between neutron guides
  - Background at instruments
Outline

- Explored interfaces:
  - Tally fit
  - Pptrac
  - SSW/SSR
  - Compile
  - Supermirror

- Validation
  - First results

- Summarizing experiences
  - Cross comparisons

- First usage
  - Guide measurements and simulation (BOA, PSI)
  - Toward $\gamma$ background estimates
**Tally fitting** (present default approach)

1. Neutron spectrum calculated with MCNP/X at the moderator surface
2. Spectrum is approximated by Maxwellian fits which serves as input to McStas.

---

**Con’s**
- Correlations (e.g. E, pos, angles) unaccounted for
- Write out at 1 surface only
- No re-entry (format is write-only)

**Pro’s**
- Fast - MCNP calculation done once-and-for-all
- Avoids licensing issues
Tally fitting (ESS update)

- Major neutron sources have their own McStas source component
- Based on the latest MCNPX ESS target station (bi-spectral) geometry, we are updating the McStas ESS source mimicking both geometry, spectra and correlations between neutron parameters
Ptrac

- MCNP/X can output an ascii file containing individual neutron states: pos, angles, energy, time & weight
- The McStas component: **MCNP_Virtual_Input** (written by E.Farhi) converts the neutron state into McStas readable and works as a source

### Pptrac format

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>3000</td>
<td>2</td>
<td>10</td>
<td>179</td>
</tr>
<tr>
<td>100</td>
<td>2</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00000E+00</td>
<td>0.28640E+00</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.43531E+00</td>
<td>-0.10000E+01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00000E+00</td>
<td>0.00000E+00</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.10000E+00</td>
<td>0.10000E+01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.33356E-02</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3000</td>
<td>3</td>
<td>110</td>
<td>179</td>
</tr>
<tr>
<td>10</td>
<td>2</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-0.20000E+00</td>
<td>0.28640E+00</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.43531E+00</td>
<td>-0.10000E+01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00000E+00</td>
<td>0.00000E+00</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.10000E+00</td>
<td>0.10000E+01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.40028E-02</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3000</td>
<td>4</td>
<td>120</td>
<td>179</td>
</tr>
<tr>
<td>100</td>
<td>2</td>
<td>0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>-0.40000E+00</td>
<td>0.28640E+00</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.43531E+00</td>
<td>-0.10000E+01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.00000E+00</td>
<td>0.00000E+00</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.10000E+00</td>
<td>0.10000E+01</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.46699E-02</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>3000</td>
<td>5</td>
<td>130</td>
<td>179</td>
</tr>
</tbody>
</table>

### Con’s
- ascii file enormous: ~0.2kB/evt
- Write out at 1 surface only
- No re-entry (format is write-only)
- Cannot run MPI

### Pro’s
- Correlations conserved (e.g. E, pos)
- Fast
SSW/SSR

- **Source Surface Read/Write** in MCNPX starts/stops simulations at a given (set of) surface(s)
- Neutron state written to binary file.
- New McStas (v2.0) components: `MCNP_Virtual_ss_Input` & `MCNP_Virtual_ss_Output`
  - read MCNPX output and write MCNPX input
- Neutron propagation started in MCNPX, continued in McStas and finalizing in MCNPX

---

- ASCII file sizeable: ~0.1kB/evt
  - Write out at selected surfaces only
  - Has not (yet) been tested with MPI

- All McStas functionality usable
  - Re-entry supported
  - Correlations conserved (e.g. E, pos)
Combined compilation

Method

- McStas surface flag introduced in MCNPX
- Neutron crossing McStas surface causes initiation of McStas simulation, based on neutron state.
- Updated neutron state returned to MCNPX

Technically difficult to make general
- Licensing issue
- Slow: MCNPX called for each neutron

Potentially very flexible (but not yet fully developed)
- All McStas functionality usable
- Re-entry supported
- Correlations conserved (e.g. E, pos)

in MCNPX input file:

......
-110 PX -0.2
-120 PX -0.4
Supermirror

- Existing implementation, introducing McStas inspired supermirrors as a surface card in MCNPX (Gallmeier et al., Nuc. Tech. 168(3))

- Reflectivity
  
  \[ R = R_0 \quad \text{if } Q < Q_c \]
  
  \[ R = R_0/2 \{ 1 - \tanh[(Q - m Q_c)/W] \} \{ 1 - a(Q - Q_c) \} \quad \text{if } Q > Q_c \]

- Ported to MCNPX 2.7
Validation setup

**Strategy**: consider dummy geometry, where the correct result is obvious:

- 20meV neutrons generated at disk and aimed 45 degree toward a perfectly reflecting 'guide wall' 1 cm away (in y)
- At z=4cm: check what comes through
- Assume vacuum in guide so that transport in McStas MCNPX should be identical

**Flux in = Flux out**
Validation results

For all interfaces:
→ Neutron energy and angle conserved (45degree, scattered twice)  ✓
Validation results

For fun: repeat after filling the guide with air

At first glance, the tails in SSW/SSR histograms surprised me. However, the tails are due to backscattering in the air outside the “McStas world”
# Cross comparison - reminder

<table>
<thead>
<tr>
<th></th>
<th>Re-entry neutrons</th>
<th>Speed</th>
<th>Single neutron trace</th>
<th>Require License</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tally</td>
<td>No</td>
<td>Fast*</td>
<td>No</td>
<td>No</td>
<td>Should try to determine validity at least once</td>
</tr>
<tr>
<td>Pptrac</td>
<td>No</td>
<td>Fast*</td>
<td>Yes</td>
<td>Yes</td>
<td>Somewhat outdated by SSW/SSR</td>
</tr>
<tr>
<td>SSW/SSR</td>
<td>Yes</td>
<td>Fast*</td>
<td>Yes</td>
<td>Yes</td>
<td>Works well</td>
</tr>
<tr>
<td>Compile</td>
<td>Yes</td>
<td>Very slow</td>
<td>Yes</td>
<td>Yes</td>
<td>Require (minor) changes to MCNPX source code</td>
</tr>
<tr>
<td>Supermirror</td>
<td>Yes</td>
<td>Slow</td>
<td>Yes</td>
<td>Yes</td>
<td>Generalizes poorly (but who cares?)</td>
</tr>
</tbody>
</table>

*) The computational heavy MCNP/X calculation can be performed once-and-for-all.
Ongoing validation / example of usage: Comparison to real data

• In collaboration with U.Filges (et al) at PSI: a ESS prototype elliptrical mirror was tested at the BOA beamline at SINQ.
• Allows cross validation of simulation approaches against real data
• Basic idea:
  → setup incl beam profile + spectrum known.
  → Intercept half beam by known material.
  → Use coupled MCNPX-McStas to describe the intensity loss.
• Status data looks promising. Starting to work on the simulations.
Ongoing validation / example of usage: Comparison to real data

- Half of the guide segment was shielded (at the exit) by different materials (polyethylene: 1.4 mm, aluminium: 1 mm, vanadium: 0.3 mm).

Measurements were done at a defocus position (10 cm behind focus plane)
Applications for shielding and $\gamma/n$ background at sample

- Simulate elliptical (ESS-like) guide in MCNPX using introduced supermirrors
  - Fast neutron/$\gamma$ background at sample
  - Shielding calculations


  i.e.:

<table>
<thead>
<tr>
<th></th>
<th>Bulk</th>
<th>Surface coating</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Ni</td>
</tr>
<tr>
<td>SiO$_2$</td>
<td>70%</td>
<td>50%</td>
</tr>
<tr>
<td>B$_2$O$_3$</td>
<td>10%</td>
<td>50%</td>
</tr>
<tr>
<td>Na$_2$O</td>
<td>8%</td>
<td>8%</td>
</tr>
<tr>
<td>CaO</td>
<td>1%</td>
<td>8%</td>
</tr>
<tr>
<td>K$_2$O</td>
<td>8%</td>
<td>8%</td>
</tr>
</tbody>
</table>

- This study was only started recently, so no reliable results yet.
Applications for shielding and $\gamma/n$ background at sample

- 1) $\gamma$ background measurement at BOA is being planned now.
- 2) Comparison with previous results
  - **NIMA 634** (2011) S130–S133. A. Szaka et al
  - Measures $\#\gamma/\#n$ with below setup (detector shielded by led → can't compare with presented results)

**Plan:** try to replica results using our developed framework → I.e. build corresponding MCNPX geometry, try to deduce source etc.
Conclusions

- Interfaces validated ✓
- Applications started....
  - Task decides which interface is more useful
Backup slides
Validation:
Fitting distributions vs. importing neutron states

- Present approach used for instrument design & physics analysis relies on a once-and-for-all fit to a spectrum.
- Clear advantages over porting individual neutrons:
  - Preliminary ESS geometry (from ESS-Bilbao), simulation 1M protons with MCNPX takes ~1K CPU hours
  - McStas CPU cost for 1M neutrons: hardly measurable in <1s

- Implicitly McStas assumes:
  - Spectrum fit is perfect
  - No correlations between: Position at moderator surface, position at guide entrance, momentum
  - No scattering between moderator surface and guide entrance

- For TMS & instrument design these assumptions are worth questioning
Validation of Tally approach: Fits

➢ No fit is ever perfect – especially not mine
Validation of Tally approach: Correlations

Stress test of the developed SSW/SSR approach:

- Simulate 1M protons hitting target wheel
- Dump all neutrons passing moderator surface to SSW output file (3.5Gb)
- In McStas, placing a PositionSensitiveDetector (PSD) ~at the surface gives:

\[ \text{Cold moderator surface} \]

\[ \text{all neutrons crossing} \]

\[ \text{relevant neutrons} \]
Validation of Tally approach: Correlations

- In McStas the procedure to provide neutron states is to connect randomly points at the moderator to points at the guide opening, and assign energy (based on a maxwellian function + modulation)
- Placing a PSD detector ~at the guide opening surface gives:

![Diagram of neutron path and detector](image)

- I.e. uniform - but long flight path of ~6m means that a point source assumption is not too far off.
- **Q**: How would the distribution look in MCNP. I.e. SSW card at 6m?

DTU Nutech, Technical University of Denmark
Validation of Tally approach: Correlations

- **A**: Flat – in the empty sense of the word:

No focus -> very few neutrons at guide
Validation of Tally approach: Correlations

Lots of other comparisons to make:

- I.e. correlations between position & energy exist. Important for moderator design etc, but perhaps not for instrument design (?). Being investigated.
Validation of SSW / SSR approach

1. Define simplest possible geometry in MCNPX
2. Run test simulation
3. Visualize events and pick one
4. Import to McStas the neutron states as recorded by SSW card
5. Run simplest possible McStas simulation from SSW input: neutron transport
6. At z=2m, write SSW & visualize
7. Based on McStas SSW resume the MCNPX simulation, and visualize
Validation: all approaches

- Test interfaces using ESS prototype guide at SINQ spallation source at PSI in summer 2012
- Allows cross validation of simulation approaches against real data
- Status (simulation-wise): Using MCAM$_1$ engineering CAD model geometry has been translated into a MCNPX readable geometry (details missing still)

1) FDS Team, China. Y.Wu, FDS Team, CAD based interface programs for fusion neutron transport simulation, Fusion Engineering and Design 84 (2009) 1987-1992
Tally contributions

- Contributions to cold spectrum

- Contributions to thermal spectrum
Revised tally approach

\[ I(x, y, E, t) \text{ from neutronics} \]

Per beamline:
\[ I_{BL}(x, y, E, t) = \frac{\Omega_{BL}(x, y)}{4\pi} I(x, y, E, t) \]
Revised tally approach

Neutron density as a function of y and polar angle \( \theta \):

- **Neutron density as a function of y and polar angle \( \theta \), all neutrons.**
  - Entries: 228160
  - Mean x: 127.8
  - Mean y: 17.26
  - RMS x: 16.2
  - RMS y: 3.62

- **Neutron density as a function of y and polar angle \( \theta \), cold neutrons.**
  - Entries: 244430
  - Mean x: 180.1
  - Mean y: 0.03273
  - RMS x: 105.8
  - RMS y: 16.1

Energy spectrum:

- Entries: 228160
  - Mean: 122.8
  - RMS: 3.43

Wavelength spectrum:

- Entries: 228160
  - Mean: 122.8
  - RMS: 3.43
Validation of MCNPX/McStas model against measurements at BOA (SINQ)

Beamline description:
- polarized neutron beam 4x15 cm
- 9.7 m free neutron flight path (straight) behind second guide section
- 5 measurement positions with three turnable axis
- CCD detector / single He-3 detector / He-3 PSD detector with TOF
- chopper/selector at position 1 (double monochromator, analyzer system)