Non-static surfaces in MCNPX: the Chopper Extension

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The Chopper Extension

Particle history

- Neutron beamlines often include moving components.
- MCNPX has stationary surfaces and static media.
- Goal of performing detailed background simulations of a beamline (guides, choppers, fast neutrons, gammas) in MCNPX.

Chopper Extension

- Non-static surfaces
  - The positions of surfaces have to be updated during execution time in small time steps.
  - Care must be taken at surface crossings.
- High-speed media
  - The cross sections and collision kinematics will depend on energy of the medium, requiring frame transformations during transport.

Standard Transport in MCNPX

Particle history in MCNPX

- Emitted source particles propagate stochastically through a geometry.

Source particle

- The particle is initialized with a weight, energy, time, cell location, emission direction, etc.

Standard Transport in MCNPX

Particle history in MCNPX

- Emitted source particles propagate stochastically through a geometry.
- Interaction type determined.

Interaction type

- $d_{\mathrm{collision}}$: distance to the next collision (from Σ_{total} and exponential distribution).
- d_{boundary}: distance to the next cell boundary.
- Others: d_{dxtran}, d_{time}, d_{ww}, d_{en}.
- A quantity, d_{min}, representing the minimum of these distances becomes the next collision type.

Standard Transport in MCNPX

Particle history in MCNPX

- Emitted source particles propagate stochastically through a geometry.
- Interaction type determined.
- Particle advances to next location and interaction takes place.

Interaction takes place

- Particle advances by d_{min} along $\vec{k}$.
- $d_{\mathrm{collision}}$: the collision kinematics are determined from $\vec{k}$, cell temperature, collision tables, etc. and the out-going particle energy and direction is found.
- d_{boundary}: the particle is processed through the surface into an adjacent cell.

Standard Transport in MCNPX

Particle history in MCNPX

- Emitted source particles propagate stochastically through a geometry.
- Interaction type determined.
- Particle advances to next location and interaction takes place.
- The process repeats.

Static geometry and materials

- The entire geometry is static throughout this process.
- Moving objects aren't handled during a history.
- Collective motion of materials is not accounted for.

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The Chopper Extension

- Handles the special case of rotation about a stationary point.
- Collective velocities of moving objects affect collision kinematics.
- The geometry is updated only when needed.

The Chopper Extension

Dynamic surface definitions

1. Surfaces(S) are defined at the origin ($S_{\mathcal{O}}$) and placed at a location (S_{world}) with a transformation at initialization.
   - $S_{\text{world}} = \boldsymbol{D}\boldsymbol{R}S_{\mathcal{O}}$
2. Surfaces are returned to the origin.
   - $S_{\mathcal{O}} = -\boldsymbol{D}_{\text{world}}\boldsymbol{R}_{\text{world}}^{-1}S_{\text{world}}$
3. The angular shift is determined.
   - $\Delta\theta = 2\pi t_{\text{curr}} f + \phi_0 - \theta_{\text{prev}}$
4. The surfaces are rotated and returned to the "world".
   - $S_{\text{world}} = \boldsymbol{D}_{\text{world}}\boldsymbol{R}_{\text{world}}\left[\boldsymbol{R}(\Delta\theta)S_{\mathcal{O}}\right]$

The Chopper Extension

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High-speed media

- The velocity at the edge of a 0.5 m radius disk spinning at 60 Hz ($\approx 200\ \mathrm{m\ s^{-1}}$) is comparable to a cold neutron ($\approx 1000\ \mathrm{m\ s^{-1}}$).
- Target-at-rest frame transformation.
  - $\vec{p}_{\text{TAR}} = \vec{p}_n - \vec{p}_t$

The Chopper Extension

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Surface crossing

- The geometry is treated as static close to a surface to avoid surface crossing errors.

Transport in MCNPX with the Chopper Extension

Particle history in MCNPX

- Emitted source particles propagate stochastically through a geometry.

Chopper Extension

- The surface definitions are updated if the particle is created in a cell that is flagged as moving, and the current cell is updated accordingly.
- The particle propagates normally through the geometry, interacting with non-moving cells as in standard MCNPX.

Transport in MCNPX with the Chopper Extension

Particle history in MCNPX

- Emitted source particles propagate stochastically through a geometry.
- The particle enters a moving cell.

Moving cells

- Any cell with surfaces that are flagged as dynamic.
- The surface definitions are updated depending on the current time.
- Only the dynamic surfaces of the current cell are updated.

Transport in MCNPX with the Chopper Extension

Particle history in MCNPX

- Emitted source particles propagate stochastically through a geometry.
- The particle enters a moving cell.
- Interaction type determined.

Interaction type

- A new distance is introduced, d_{motion}, which is found from the user specified time limit and the neutron velocity.
- The collective velocity is used to transform the particle into the target-at-rest system before determining the cross section, and thus before determining the mean-free-path and $d_{\mathrm{collision}}$.

Transport in MCNPX with the Chopper Extension

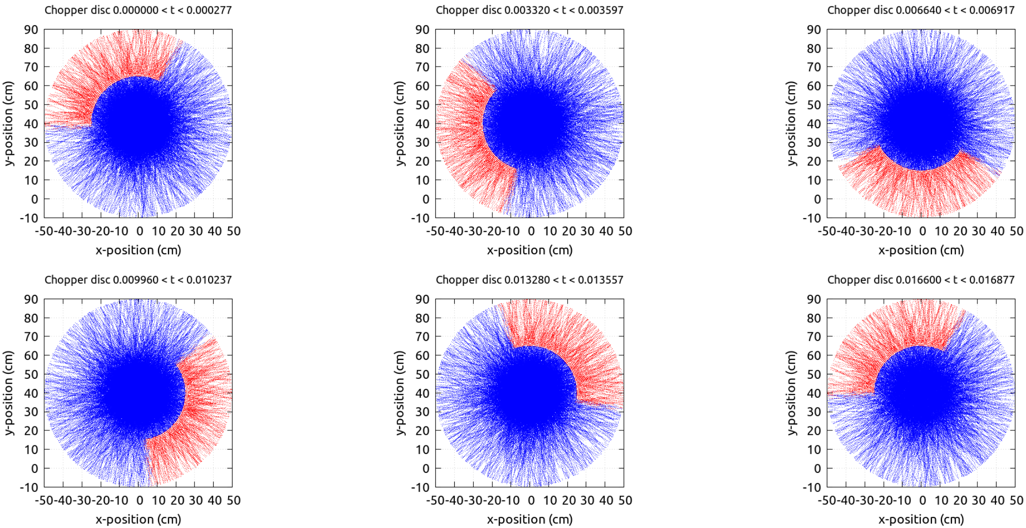
Particle history in MCNPX

- Emitted source particles propagate stochastically through a geometry.
- The particle enters a moving cell.
- Interaction type determined.
- Particle advances to next location and interaction takes place.

Interaction takes place

- d_{motion}: the particle advances by a small step and returns to update the surface definitions again.
- $d_{\mathrm{collision}}$: the particle is transformed into the target-at-rest system, collision kinematics are calculated as in standard MCNPX, and then the particle is transformed back into the laboratory system.

Neutron tracks in a chopper



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Phenomena

Kinematics

- Collective velocity of spinning object affects scattered neutron beam direction.
- Energy of nuclei in medium affects the cross section for collisions.
  - Dragging of neutron trajectories along motion direction.
  - Asymmetric field of neutrons outside a spinning object.
  - Spectrum of scattered is significantly changed.

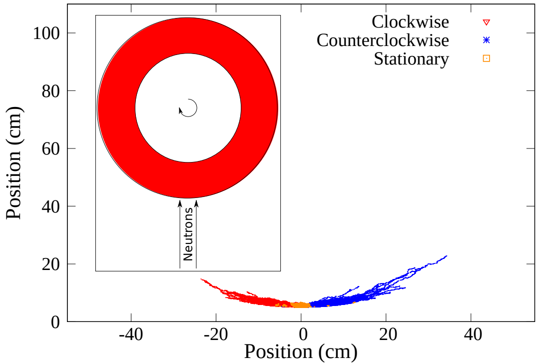
Time dependent geometries

- Can study time dependent phenomena (choppers).
- Cold neutron beam can be propagated down a beamline while preserving background information (fast neutrons, gammas).

Dragging along the direction of motion

Particle history

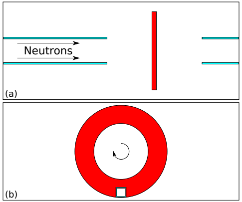
- Transformation into target-at-rest frame takes place before determining cross sections and collision kinematics.
- Consider neutrons incident into edge of thick polyethylene disc spinning at 600 Hz.

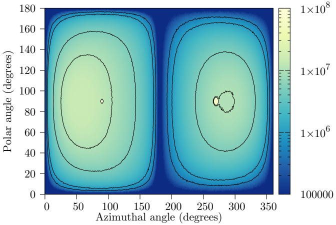


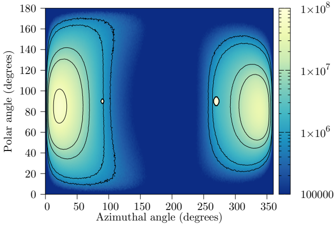
Time dependent geometries

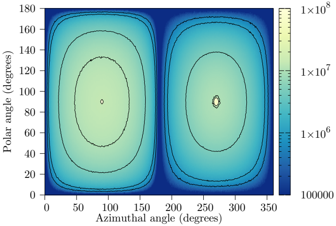
- Neutrons will, in general, carry extra momentum in the direction of momentum after collision in a moving medium.

Asymmetric field of scattered neutrons







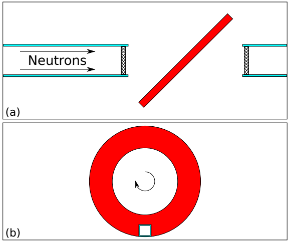


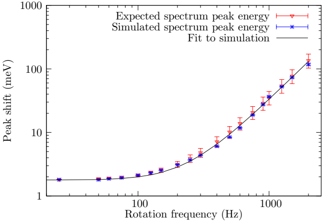
Integrals of 85° angular regions

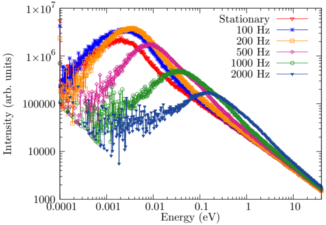
Region	0 Hz	60 Hz CW	600 Hz CW
Upstream left	32.9	41.1	64.6
Upstream right	32.9	24.4	1.4
Downstream left	17.1	12.9	0.6
Downstream right	17.1	21.6	33.4

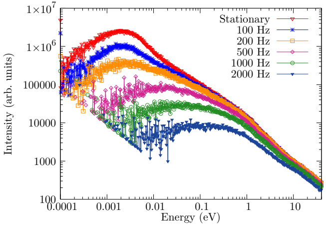
- Mono-energetic source of 5 Å neutrons incident on the polyethylene disc with no rotation, and spinning at 60 Hz and 600 Hz.

Shift in the energy spectrum





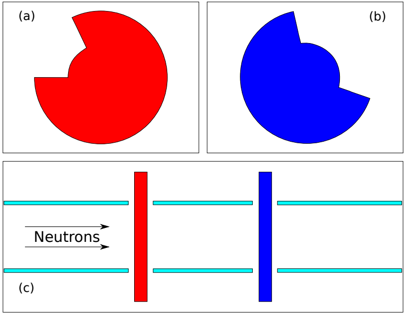


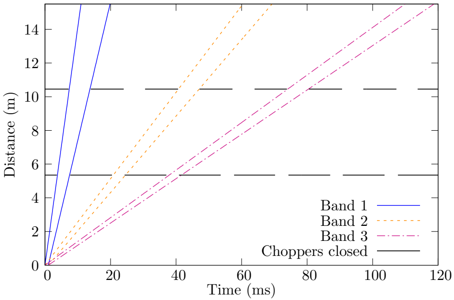


Spectral shift for moving media

- A beam of 100 eV neutrons incident on a 20 K polyethylene disc, tallying neutron energy spectrum downstream (left) and upstream (right).
- Energy shift of the peak due to the kinetic energy of the hydrogen atoms, $E_{\mathrm{H}}(f) = 2m_{\mathrm{H}}(\pi f r)^2$.

Bandwidth chopper simulation





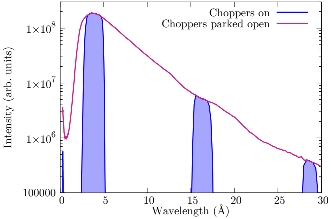
Two chopper configuration

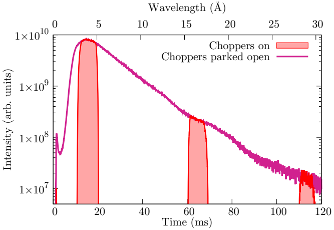
- Band pass of 2 Å centered at 3.8 Å when operated at 60 Hz.
- 5 Hz source illustrates frame overlap.

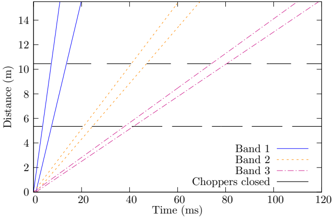
Time schedule

- TOF reconstruction of the energy spectrum should be possible.

Bandwidth choppers







Simulation results

- Good agreement between energy tallied spectrum(left) TOF converted spectrum (center)
- Consistent frame overlap locations between the TOF spectrum (center) and the time schedule (right).

Conclusions

The Chopper Extension

- Time dependent surfaces and high-speed media can be studied in MCNPX with the Chopper Extension.
- Significantly different neutron spectra through spinning objects compared to static objects.

Future work

- Moving media inside static surfaces (eg. flowing fluid) and other kinds of motion (eg. linear translation)would be straightforward to build into the existing framework.
- Along with other code extensions (SANS, guides, single crystals), the Chopper Extension is part of a powerful suite of tools for performing detailed simulations of a neutron beamline for background studies.

Thank you!