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Title: Adding Delta Tracking to the MCNP Code

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Adding Delta Tracking to the MCNP Code

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XCP-3 Monte Carlo Codes

MCNP User Symposium
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Outline

Theory

MCNP Implementation

Testing

Section 1

Theory

Background & Motivation

Within the MCNP code, particles are tracked using "surface-to-surface" tracking:

- Break geometry into regions with constant materials.
- Sample distance to collision δ_c, compute distance to surface, δ_s
- If $\delta_c > \delta_s$, move to surface
- Else, move to collision and sample collision

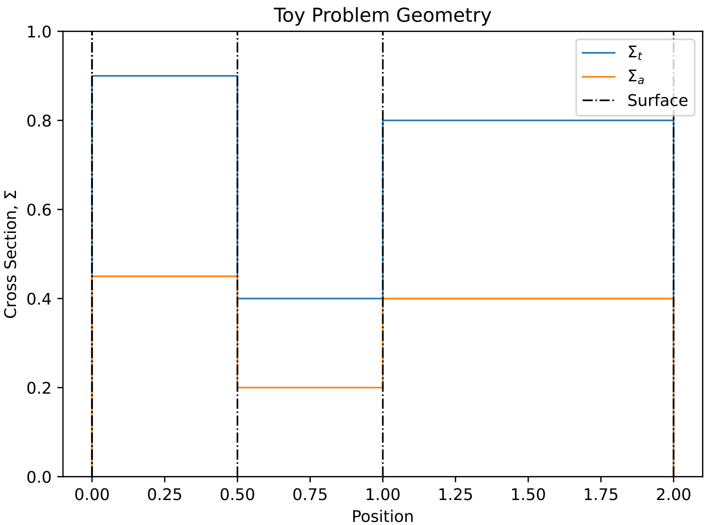
Implementation is easy, as constant materials means constant collision probability (Σ_t), and the distance sampling is analytic:

$$\delta_c = \frac{-\ln(\xi)}{\Sigma_t}$$

Similarly, constant materials means tallies have a constant multiplier over each track, and one can use track-length tallies (which are used extensively within the MCNP code).

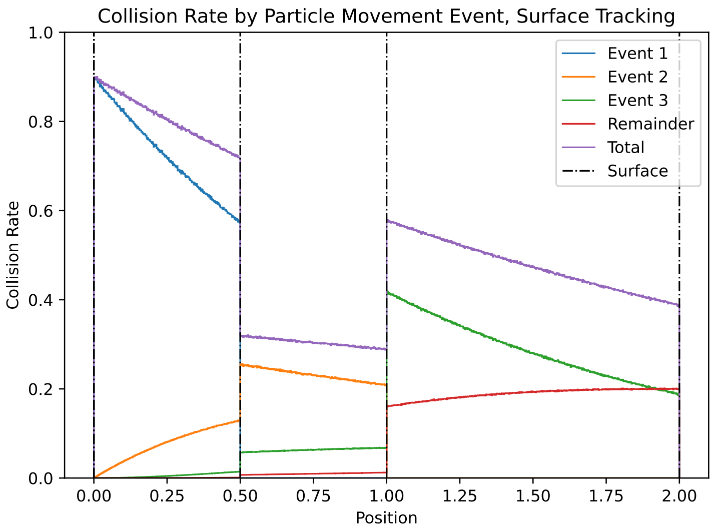
Toy Problem

Let us consider a toy problem for demonstrating algorithms.



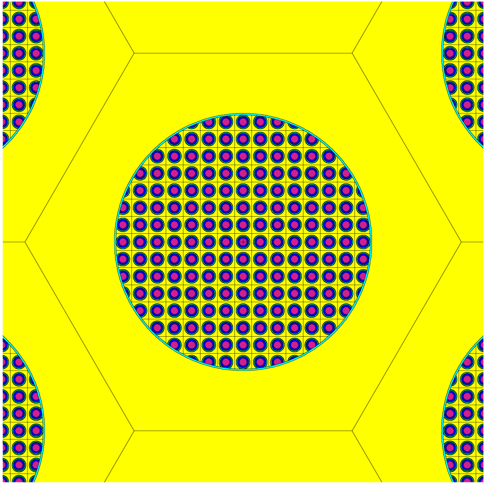
Surface Tracking

Event: any iteration of the transport loop (here, collision or surface crossing), requiring data lookups and resampling.



TRISO Problems

- TRISO fuel is very small
- A full reactor can have well in excess of 5 billion surfaces
- Every crossing requires many computations
- This results in poor performance



TRISO Fuel Element
(cylinder is 1.5 cm across)

Alternatives

- Numerical Methods
  - Can handle continuously varying materials well
  - Discontinuities require either stopping the particle or taking many steps near the discontinuity

- Delta Tracking
  - Focus of this talk
  - Can handle discontinuous materials
  - Used in the Serpent Monte Carlo code

The Delta Tracking Method

1. Add to the collision probability Σ_t a probability of not colliding Σ_{nc}.
2. Select Σ_{nc} such that $\Sigma_t + \Sigma_{nc}$ is constant and Σ_{nc} is non-negative. $\Sigma_t + \Sigma_{nc}$ is now called the "Majorant", Σ_m.
3. Track with this new cross section. Distance is now:

$$\delta_c = \frac{-\ln(\xi_1)}{\Sigma_m}$$

4. Move particle δ_c.
5. Randomly sample if a collision was real or not:
   - 5.1 If $\xi_2 < \frac{\Sigma_t}{\Sigma_m}$, collide
   - 5.2 Else, leave particle as-is.

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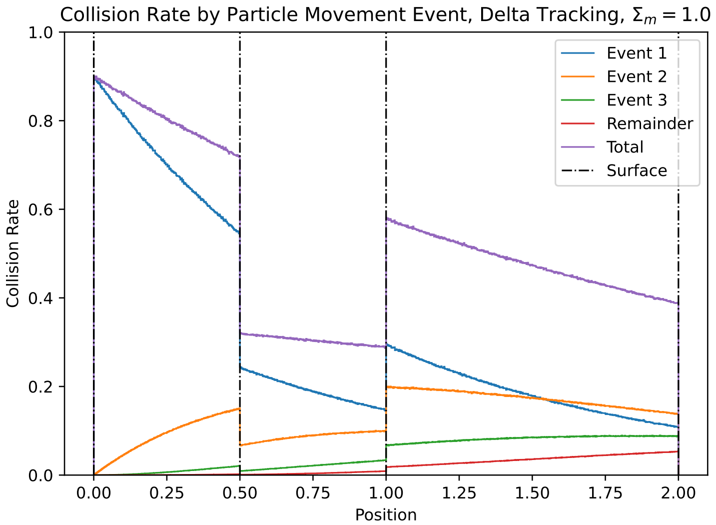
Delta Tracking

Using delta tracking, one notes that every part of the geometry is tallied in the first event, and fewer events are needed to make it through on average.



Advantages and Disadvantages to Delta Tracking

Advantages:

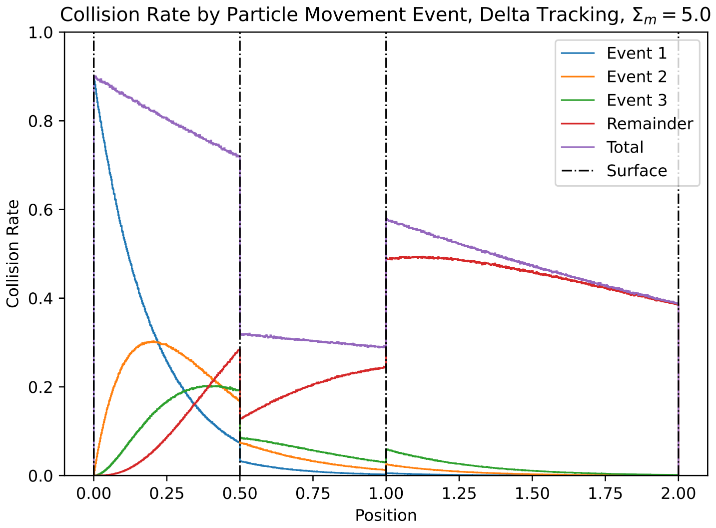
- Adding more surfaces does not affect performance (aside from possibly increasing cell-at-point-of-collision lookup time)

Disadvantages:

- A large majorant will cause more collisions, harming performance
  - Burnable absorbers are key culprit
- Cannot use track-length tally estimators for most values of interest without issue
  - Exception is flux tallies in a structured mesh, where distance in cell is easy to compute and there is no discontinuous weighting function

Large Majorant Example

If the majorant is increased (say, due to burnable absorbers), events occur more often, reducing efficiency.



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Tallies

As mentioned earlier, delta tracking does not support track-length estimators in most configurations:

- For cell tallies, would need to determine if each track entered a cell and for how long
- For reaction rate tallies, would need the same for materials

Computing this information would nullify the delta tracking advantage. So, instead, at every event, we tally:

$$\text{score} = \frac{\text{weight} \times \text{multiplier at event}}{\Sigma_m}$$

(Pseudo-)collision tallies tend to have a larger variance than track-length tallies, particularly as tally domain size shrinks.

Tally Comparisons

As the tallies get finer, track-length tallies statistically outperform collision tallies. Ratios are exaggerated by being 1D.

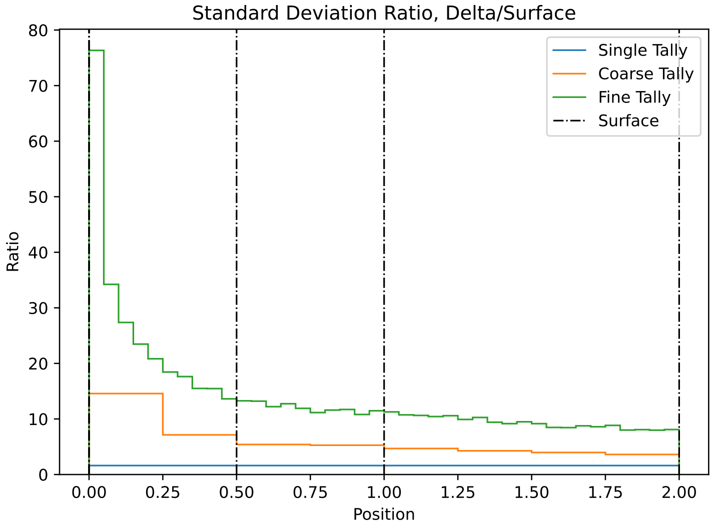


Figure of Merit

While the variance of the tallies may be higher, if the simulation runs faster, you can run more particles to make up for it.

$$\text{variance} \propto \frac{1}{\text{number of simulated particles}} \propto \frac{1}{\text{time}}$$

Based on the above relationship, $(\text{variance} \times \text{time})$ should be roughly constant for any given algorithm. So, the figure of merit for Monte Carlo, FOM is given by:

$$\text{FOM} = \frac{1}{\sigma^2 t}$$

The ratio of the FOM between algorithms shows, roughly, how much more efficient one algorithm is compared to another.

Section 2

MCNP Implementation

Computing the Majorant

There are several ways one can compute the majorant:

1. Get the global maximum Σ_t
2. Create a function such that $\Sigma_m(E) \geq \Sigma_t(E)$ for all positions

This latter form is made possible by the fact that neutrons and photons do not change energy except during collision (in the physics implemented in MCNP).

Making it a function of energy is beneficial. As shown earlier, a large majorant reduces efficiency. This form will reduce Σ_m over most energies.

Data Components

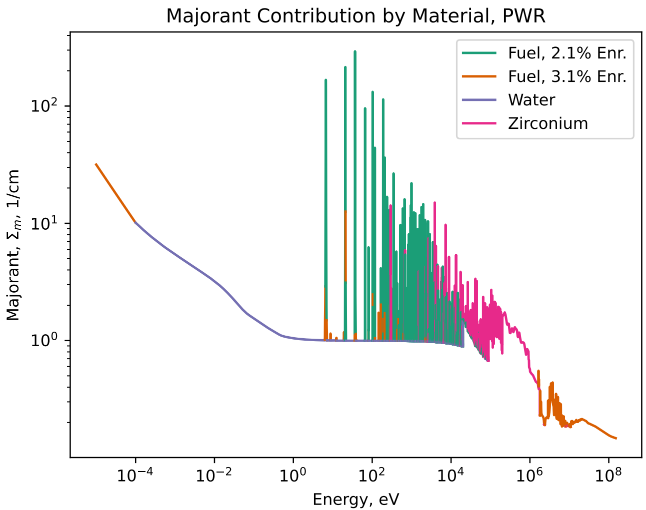
For each particle, the majorant must take into consideration all contributions. In the MCNP code, these are:

- Neutrons
  - Basic reaction rates - linear-linear representation
  - Unresolved resonances - several possible representations
  - $S(\alpha, \beta)$ - two components are linear-linear, one is piecewise functions proportional to $1/E$
- Photons
  - Photoatomic - log-log representation
  - Photonuclear - linear-linear representation

$\Sigma_m(E)$ was chosen to be linear-linear interpolated, as it makes several datasets trivial and the rest can be quickly approximated as linear-linear.

Majorant

The majorant is then computed during simulation load:



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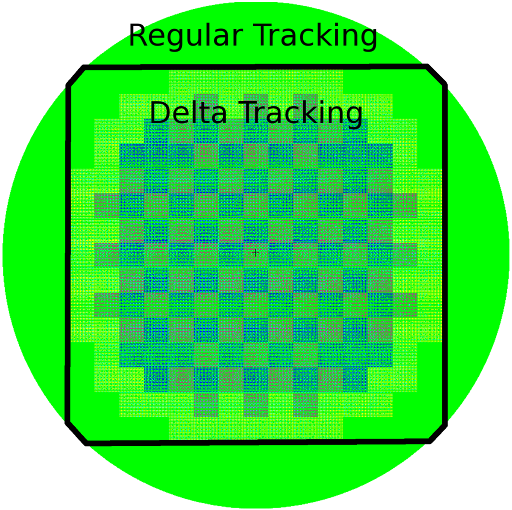
Transport Modifications

- A hybrid approach was used:
  - If in a “delta-tracking universe”, use the delta tracking code path
  - If not, use the regular surface-to-surface code path
- This allows one to get performance benefits inside of a core, while still allowing surface tallies in the perimeter.



Gaps in Implementation

The MCNP code has decades of features implemented assuming surface-to-surface tracking. To support everything in the first pass would be folly.

The following are known to not work with delta tracking at this time:

- Most variance reduction - many need rederiving/reconsidering
- Unstructured/structured mesh geometry - uses a completely different code path
- All non-neutron/photon particles - most of the benefits are invalid for charged particles, for example

Other particles are still allowed, they just ignore the delta tracking flag.

Section 3

Testing

Testing

With such a radical change in the transport algorithm, care needed to be taken to ensure things did not break.

Generated two k-eigenvalue test problems:

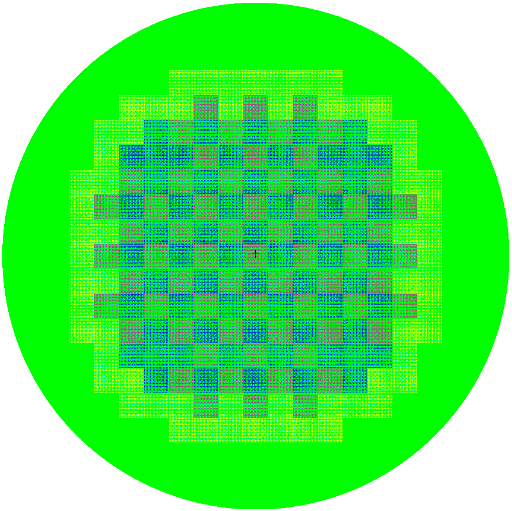
1. A 2D PWR
2. A simplified TRISO reactor

Configuration:

- Each run 50 times, with and without delta tracking
- Neutrons, photons, and photonuclear physics was enabled
- Cell tallies performed in several cells
- FMESH energy deposition tallies performed over whole core

2D PWR

- 1,000,000 particles per generation
- 100 inactive generations
- 200 active generations
- ENDF/B-VIII.0 data
- 15×15 FMESH tallies
- Tallies in fuel, clad, water



PWR Layout

2D PWR Tallies

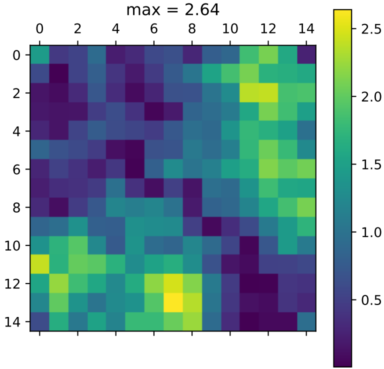
Value	δ, in std-dev	FOM Ratio
k-eigenvalue	0.50	1.65
Neutron Σ_a, fuel	0.45	1.34
Neutron Σ_a, clad	1.22	0.70
Neutron Σ_a, water	0.04	1.28
Photon Σ_t, fuel	0.74	1.54
Photon Σ_t, clad	0.94	1.14
Photon Σ_t, water	1.37	1.67

In all cases, the difference in units of standard deviations does not indicate any issues with the implementation. Further, the maximum relative error between the two transport modes was 5.4×10^{-5}, putting a tight bound on any error hidden by statistics.

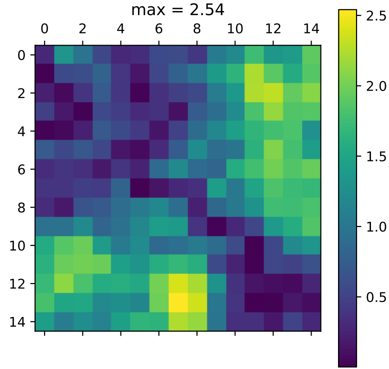
Performance wise, the figure of merit increased a moderate amount for most tallies. The cladding, being quite thin, falls afoul of the increased variance for small regions issue.

2D PWR FMESH Accuracy

Difference between tallies, in units of standard deviations



(a) Neutrons

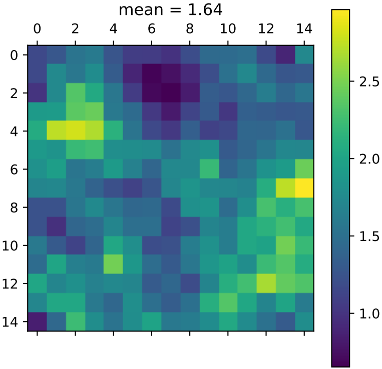


(b) Photons

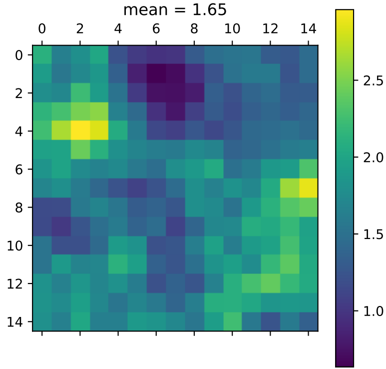
Both FMESH tally results show no unexpected discrepancies.

2D PWR FMESH FOM

Ratio of figure of merit, delta over surface-to-surface



(c) Neutrons



(d) Photons

Delta tracking improved performance moderately, but it was spatially non-uniform.

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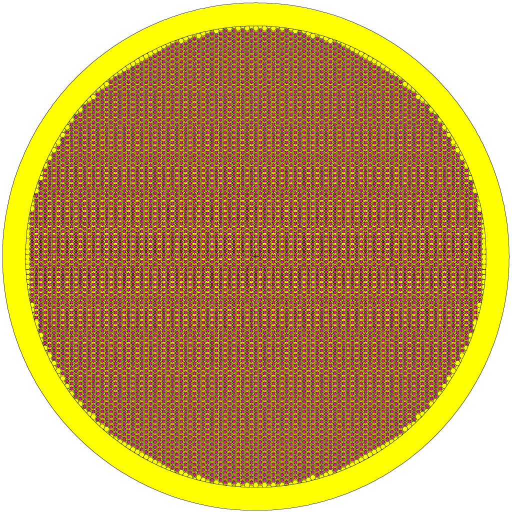
TRISO Model

- 100,000 particles per generation
- 100 inactive generations
- 200 active generations
- ENDF/B-VIII.0 data
- 22×22 FMESH tallies
- Tallies in fuel, TRISO layers



TRISO Reactor Layout

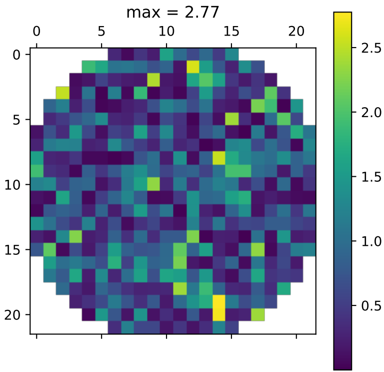
TRISO Model Tallies

Value	δ, in std-dev	FOM Ratio
k-eigenvalue	0.41	13.49
Neutron Σ_a, fuel	1.42	13.39
Neutron Σ_a, layer 1	0.71	3.77
Neutron Σ_a, layer 2	0.86	0.86
Neutron Σ_a, layer 3	0.03	4.58
Neutron Σ_a, layer 4	0.13	1.63
Photon Σ_t, fuel	0.30	19.78
Photon Σ_t, layer 1	0.80	18.78
Photon Σ_t, layer 2	1.03	8.55
Photon Σ_t, layer 3	0.25	8.75
Photon Σ_t, layer 4	0.58	8.73

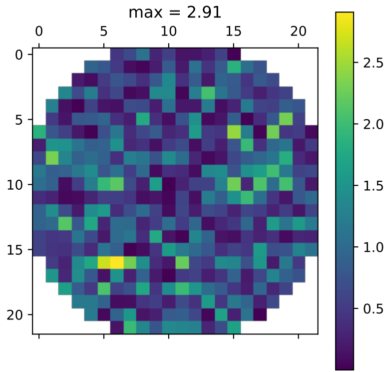
No indication of errors in the implementation. The maximum relative error was 4.8×10^{-4}. FOM improvements are much larger than the PWR results for most of the geometry.

TRISO FMESH Accuracy

Difference between tallies, in units of standard deviations



(e) Neutrons

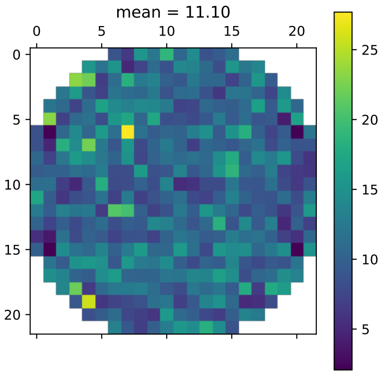


(f) Photons

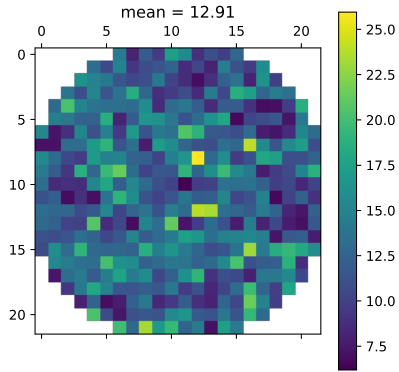
Still no indication of abnormal behavior.

TRISO FMESH FOM

Ratio of figure of merit, delta over surface-to-surface



(g) Neutrons



(h) Photons

Performance improvements are more uniform and of larger magnitude than the PWR simulation.

Summary

- Small improvements in regular geometries like a PWR
- Large performance improvements in fine geometries like TRISO reactors
- Testing showed no indication of implementation error in any test performed
- Further testing and cross-feature checking will be done for a future production release of the MCNP code.

Acknowledgements

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