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Title: Functional Expansion Tallies Using MCNP6 PTRAC Files

Author(s): Vaquer, Pablo Andres
Rising, Michael Evan
Weaver, Colin Andrew

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Functional Expansion Tallies Using MCNP6 PTRAC Files

Pablo A. Vaquer, Michael E. Rising, and Colin A. Weaver

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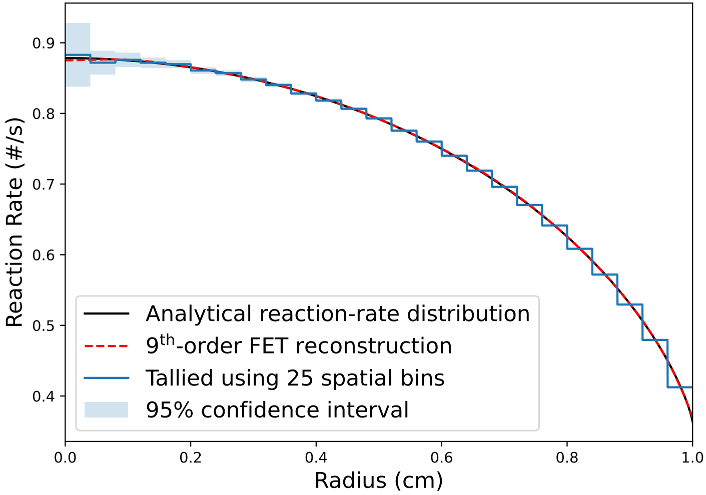
Motivation for Using Functional Expansion Tallies

- Accuracy is vital for many radiation transport applications
- Monte Carlo (MC) codes are the most accurate, but they are expensive for fine meshes
- Functional Expansion Tallies (FETs) yield smoother, lower-variance results with far fewer degrees of freedom



Theory: Functional Expansion Tallies (FETs)

- An FET expands a quantity of interest in a chosen basis
- Step 1: A Monte Carlo simulation tallies spatial moments of the quantity of interest
- Step 2: After the simulation, the moments are used to reconstruct a functional distribution

$$\mathcal{R}(r) \approx \sum_{m=0}^{N} a_m \, b_m(r) \tag{1}$$

$\mathcal{R}(r)$	functional expansion of the reaction rate
r	position within a sphere
a_m	m^{th} expansion coefficient
$b_m(r)$	m^{th} basis function evaluated at r

Spatial Moments in Spherical Geometry

Recall that "Step 1" in the FET procedure involves tallying spatial moments of the reaction rate in Monte Carlo

- The analytical expression for the spatial moment of the reaction rate is

$$\langle \mathcal{R} \rangle_n = 4\pi \int_0^R \mathcal{R}(r)\, b_n(r)\, r^2\, dr \tag{2}$$

$\langle \mathcal{R} \rangle_n$	n^{th} spatial moment of reaction rate
$\mathcal{R}(r)$	true (unknown) reaction-rate distribution
$b_n(r)$	n^{th} basis function, evaluated at radius r
r	radial distance from the sphere's center, $r = \sqrt{x^2 + y^2 + z^2}$
R	sphere's radius

Approximate Spatial Moments in Spherical Geometry

After substituting the functional expansion $\mathcal{R}(r) = \sum_{m=0}^{N} a_m \, b_m(r)$ into the spatial-moment integral, $\langle \mathcal{R} \rangle_n = 4\pi \int_0^R \mathcal{R}(r) \, b_n(r) \, r^2 \, dr$, the n^{th} moment becomes

$$\langle \mathcal{R} \rangle_n \approx \sum_{m=0}^{N} a_m \, 4\pi \int_0^R b_m(r) \, b_n(r) \, r^2 \, \mathrm{d}r \tag{3}$$

- $\langle \mathcal{R} \rangle_n$ approximate n^{th} spatial moment of the reaction rate
- a_m expansion coefficients (unknowns to be solved)
- $b_m(r)$, $b_n(r)$ basis functions evaluated at radius r
- r radial distance from sphere's center, $r = \sqrt{x^2 + y^2 + z^2}$
- R sphere's radius

Monte Carlo collision estimator

The Monte Carlo collision estimator for spatial moments of reaction rate is

$$\langle \mathcal{R} \rangle_n \approx \frac{1}{W} \sum_{i \in I} b_n(r)\, w_i \,, \tag{4}$$

$\langle \mathcal{R} \rangle_n$	is the n^{th} spatial moment of the reaction rate, $\mathcal{R}$
$b_n(r)$	n^{th} basis function, evaluated at r
r	radial distance from sphere's center, $r = \sqrt{x^2 + y^2 + z^2}$
w_i	particle weight for the i^{th} collision
W	total starting weight of all particles
I	set of all collision events within a volume

Solving for Expansion Coefficients

Linear system for the coefficients a_m:

$$\underbrace{\begin{bmatrix} \mathcal{I}_{00} & \mathcal{I}_{01} & \cdots & \mathcal{I}_{0N} \\ \mathcal{I}_{10} & \mathcal{I}_{11} & \cdots & \mathcal{I}_{1N} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{I}_{N0} & \mathcal{I}_{N1} & \cdots & \mathcal{I}_{NN} \end{bmatrix}}_{\mathbf{I}} \underbrace{\begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{bmatrix}}_{\vec{a}} = \underbrace{\begin{bmatrix} \langle \mathcal{R} \rangle_0 \\ \langle \mathcal{R} \rangle_1 \\ \vdots \\ \langle \mathcal{R} \rangle_N \end{bmatrix}}_{\vec{M}}$$

For spherical geometry, the matrix elements are

$$\mathcal{I}_{mn} = 4\pi \int_0^R b_m(r)\, b_n(r)\, r^2 \, \mathrm{d}r$$

- $\vec{M}$ spatial moments tallied during the MC run
- $\mathbf{I}$ geometry-dependent moment matrix (analytic for chosen basis)
- $\vec{a}$ unknown expansion coefficients (solved by $\mathbf{I}^{-1}\vec{M}$)

Collision-Based FET Workflow

1. MCNP6.3.1 records every collision in a PTRAC file (position, weight, etc.).
2. Python package tallies moments using basis functions $b_n(r) = r^n$
3. Assemble linear system $\mathbf{I}\vec{a} = \vec{M}$
4. Solve for $\vec{a}$ and evaluate $\mathcal{R}(r)$ on a fine grid

Python Implementation of Collision-Based FETs

```python
import h5py
import numpy as np
import matplotlib.pyplot as plt

ptrac_file = "ptrac.h5"
size = 1
order = 9
nps = 1e8

print("Loading ptrac data")
h5file = h5py.File(ptrac_file, "r")
data = [h5file["ptrack/Collision"][i] for i in
        ["x", "y", "z", "weight"]]
print("Done!\n")

# Convert coordinates of collisions to "r"
x, y, z, weights = data
r = np.sqrt(x**2 + y**2 + z**2)

print("Tallying moments and building matrix")
moments = np.zeros(order+1)
matrix = np.zeros((order+1, order+1))
for m in range(order+1):
    moments[m] = np.sum(weights * r ** m)
    moments[m] /= nps
    for n in range(order+1):
        matrix[m, n] = 3/(3+n+m) * size ** (n+m)
print("Done!\n")
```

```python
# Replace last moment with boundary condition
matrix[-1, :] = 0
matrix[-1, 1] = 1
moments[-1] = 0

print("Computing FET coefficients")
coeffs = np.linalg.solve(matrix, moments)
print("Done!\n")

# Create spatial grid for plot
x_grid = np.linspace(0, size, int(1e6))

print("Computing reaction-rate distribution")
reaction_rates = np.zeros_like(x_grid)
for n in range(order+1):
    reaction_rates += coeffs[n] * x_grid ** n
print("Done!\n")

# Plot FET reaction rate distribution
plt.plot(x_grid, reaction_rates)
plt.xlabel(r"Radial Distance (cm)")
plt.ylabel(r"Reaction Rate (#/s)")
plt.show()
```

Download here:

Analytical Verification Problem

Analytical Problem Description:

- Sphere ($R = 1$) in a vacuum
- Partially scattering medium ($\Sigma_s = \Sigma_a = 0.5$)
- Isotropic source uniformly distributed in sphere ($Q = 1$)
- Reference analytic solution derived during last year's MCNP sympsoium:
  - C. A. Weaver and M. E. Rising, "Studying the Random Number Generators in MCNP6 using an Analytic Benchmark," Tech. Rep. LA-UR-24-28791, Los Alamos National Laboratory, Los Alamos, NM, USA (Aug. 2024)

Simulation Description:

- MCNP6.3.1, simple_ace.pl, and Python post-processor
- 100 million particle histories
- PTRAC file with only collision events
  - $\sim$ 80 million collisions

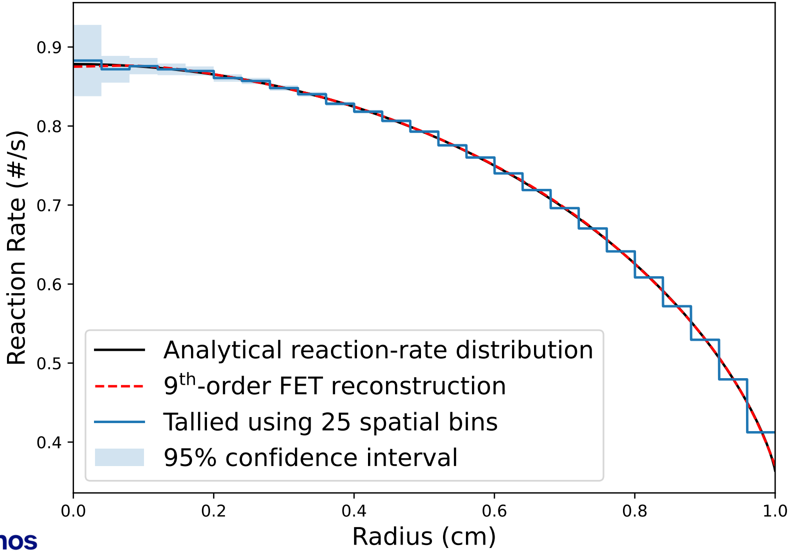
MCNP6 Input File for Analytical Verification Problem

```
Analytical sphere problem
1   100     1     -10      imp:n=1
2   0              10      imp:n=0

10    so     1

sdef rad=d1
si1 0 1.       $ 0 to 1 cm
sp1 -21 2      $ power law sampling for sphere
sb1 -21 -0.5   $ just for variance reduction
xs100   99001.01c 1e+06    99001.01c  0 1 1 16  0 0 2.5301e-08
m100    99001.01c 1  $ generated by simple_ace.pl
nps 1e8
ptrac file=hdf5 flushnps=1e7 event=col  $ only save collisions
phys:n j 1000 $ analog capture below 1 GeV
```

Analytical Verification Results



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FET solution is over $10\times$ better than than best binned tally!

FET Order	L2 Error Norm
1	1.78×10^{-1}
2	2.49×10^{-2}
3	1.03×10^{-2}
4	4.82×10^{-3}
5	2.53×10^{-3}
6	2.00×10^{-3}
7	1.21×10^{-3}
8	8.84×10^{-4}
9	7.49×10^{-4}
10	1.14×10^{-3}
20	1.70×10^{-3}
30	1.53×10^{-3}

Blue font = Minimum error

# Spatial Bins	L2 Error Norm
10	1.96×10^{-2}
25	8.23×10^{-3}
100	1.43×10^{-2}
250	3.27×10^{-2}
1000	5.19×10^{-2}
2500	1.13×10^{-1}
10000	1.91×10^{-1}

Blue font = Minimum error

BeRP-Ni Benchmark

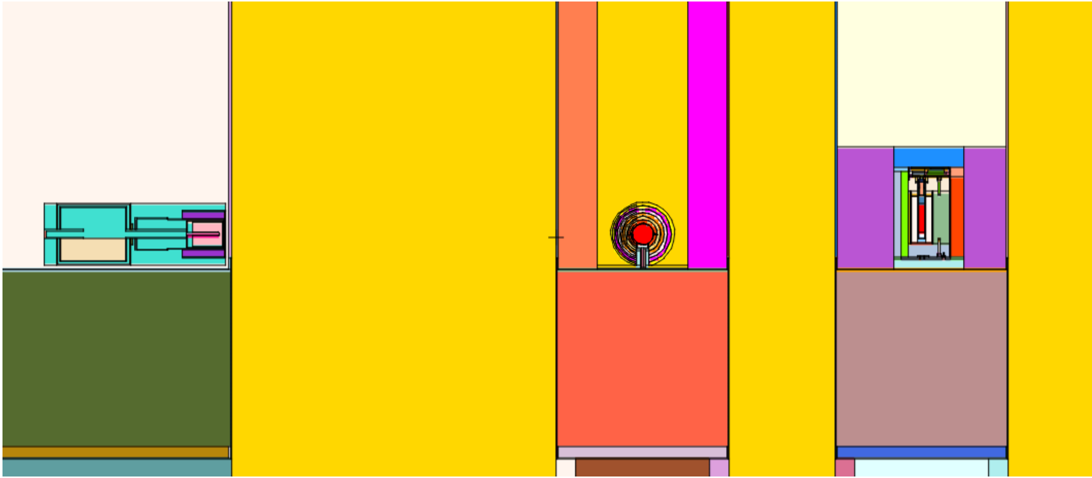
Problem Description

- Sphere of plutonium in an asymmetrical experimental setup
- Uniformly distributed spontaneous-fission source

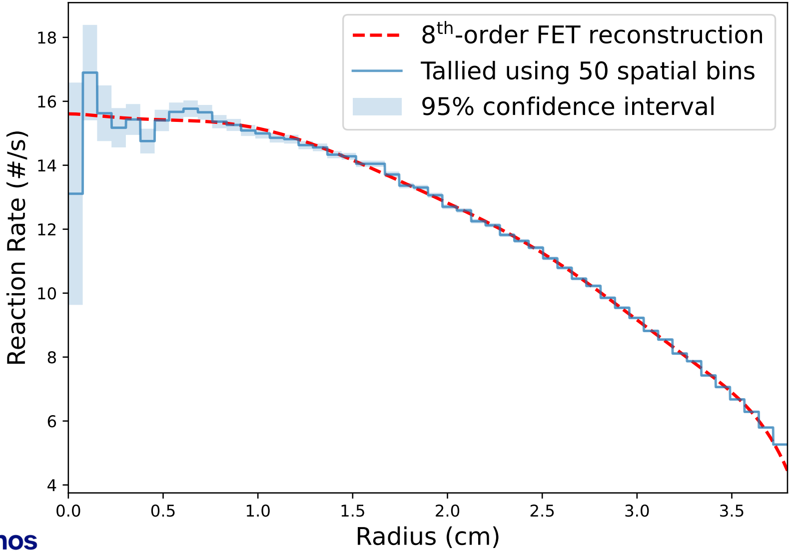
Simulation Description

- MCNP 6.3.1 with Python post-processor
- 2 million particle histories
- PTRAC file containing only collision events
  - $\sim$1.47 billion collisions

MCNP6 Geometry for BeRP-Ni Experiment



BeRP-Ni Benchmark Results



Conclusions & Future Work

Conclusions:

- Collision-based FETs reconstruct smooth reaction-rate fields with 10$\times$ lower error than conventional bins
- Post-processing overhead is negligible relative to MCNP6 run time
- Framework generalizes to any tally-able quantity and geometry
- Slab and cylindrical geometry FETs will be presented at the 2025 American Nuclear Society Winter Meeting in Washington D.C.

Future Work:

- Integrate into MCNP Python package
- Propagate statistical uncertainties to provide confidence intervals
- Embed FET logic directly into MCNP source code

References

1. D. P. Griesheimer, *Functional Expansion Tallies for Monte Carlo Simulations*, Doctoral Dissertation, University of Michigan, (2005).
2. J. A. Kulesza *et al.*, “MCNP® Code Version 6.3.0 Theory & User Manual,” Tech. Rep. LA-UR-22-30006, Rev. 1, Los Alamos National Laboratory, Los Alamos, NM, USA (Sep. 2022).
3. C. A. Weaver, P. A. Vaquer, & M. E. Rising, “A Verification Benchmark for One-Speed Transport in One-Dimensional Cylindrical Geometry,” American Nuclear Society Winter Meeting - Washington D.C., USA (Nov. 2025).
4. C. A. Weaver & M. E. Rising, “Studying the Random Number Generators in MCNP6 using an Analytic Benchmark,” Tech. Rep. LA-UR-24-28791, Los Alamos National Laboratory, Los Alamos, NM, USA (Aug. 2024).
5. B. Richard, J. D. Hutchinson, M. A. Smith-Nelson, T. E. Cutler, A. Sood, “IER-161, BeRP Ball Reflected by Nickel Benchmark Evaluation,” Tech. Rep. LA-UR-14-21929, Los Alamos National Laboratory, Los Alamos, NM, USA (2014).

Questions?

Thank you!

vaquer@lanl.gov