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Improvements to Contributions from Neutron Inelastic Scattering for Next-Event Estimators in MCNP® Software

Jeremy Sweezy

4th Annual 2024 MCNP® User Symposium
Aug 20, 2024

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Conclusions for the Impatient - Spoiler Alert!

- Minor corrections in MCNP® 6.3.1 for inelastic neutron scattering contributions to Point Det. / DXTRAN spheres
- Average users won't notice. Nuclear data nerds might.
  - Inelastic cross section generally much smaller than elastic cross section
  - Energy range of the corrections:
    - $\Delta E = -Q/(A * (A-1))$
    - H-1, He-3, He-4 have no inelastic reactions
    - Only appreciable for Deuterium (H-2) and Tritium (H-3)
    - Small energy range, $-Q \times$ (10's keV), for small mass targets ($3 < A < 33$)
    - Tiny energy range, $-Q \times$ ($<$ 1 keV), for large mass targets ($A > 33$)

What is a Next-Event Estimator?

- In MCNP nomenclature, a Next-Event Estimator (NEE) is termed a point detector, or `F5` tally
- `FIP`, `FIC`, and `FIR` tallies are arrays of NEEs
- DXTRAN (`DXT`), Deterministic Transport, also uses NEE scattering physics

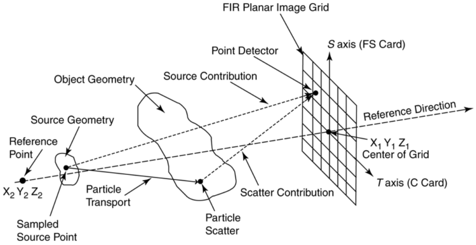
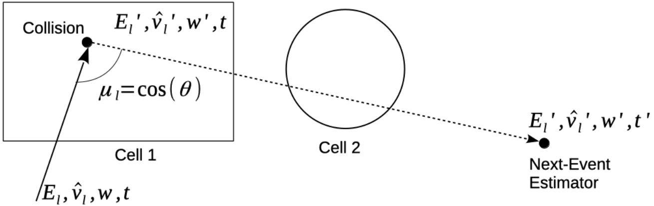


Diagram of a FIR (Flux Image Radiograph) tally.

NEE Energy from Neutron Inelastic Scattering



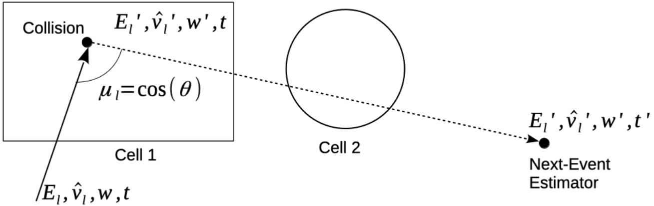
$$(E'_{l\pm})^{1/2} = \left[\frac{\mu_l (E_l)^{1/2}}{A+1} \pm \left(\frac{\mu_l^2 E_l}{(A+1)^2} + E'_c - \frac{E_l}{(A+1)^2} \right)^{1/2} \right] \quad (5.14)$$

Particle-Transport Simulation with the Monte Carlo Method

L. L. Carter and E. D. Cashwell
Los Alamos Scientific Laboratory

"..the lower root E'_{l-} can usually be ignored without introducing appreciable error.' [1]

NEE Energy from Neutron Inelastic Scattering



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NEE Energy from General Neutron Scattering

- Generalized equation (moving and non-moving target, elastic and inelastic scattering) for outgoing neutron energy in the LAB frame [2, 3]:

$$E'_{l\pm} = E_{cm}\left[\mu_l \pm D\right]^2$$

For a stationary target: $E_{cm} = \frac{E_l}{(A+1)^2}$ (Specific Energy of COM System)

$$D = \sqrt{\mu_l^2 - \left(1 - \frac{E'_c}{E_{cm}}\right)}$$ (This is the $\sqrt{\text{discriminate}}$)

- The outgoing energy in the COM frame, E'_c, is:
  - provided by nuclear data for inelastic scattering
  - provided by kinematics for elastic scattering ($E'_c = E_c$)

NEE Weight from General Neutron Scattering

- The outgoing weight is the original weight multiplied by the differential angular probability,

$$w' = wp(\mu_l)$$

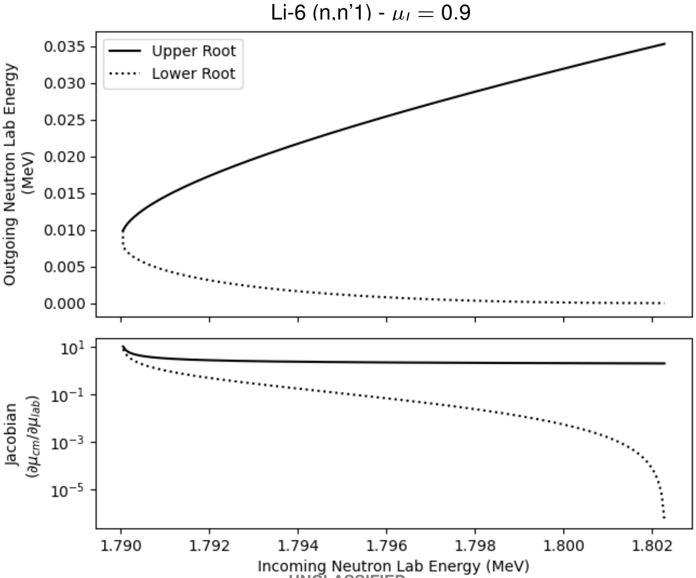
- The Jacobian ($\partial\mu_c/\partial\mu_l$) is used for conversion of the differential angular probabilities from the center-of-mass (COM) to laboratory frame (LAB):

$$p(\mu_l) = p(\mu_c)\partial\mu_c/\partial\mu_l$$

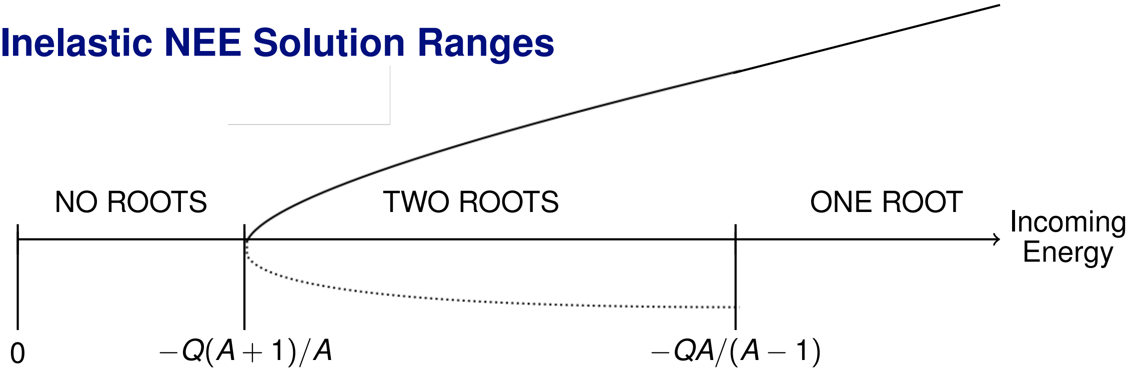
- And an expression for the Jacobian ($\partial\mu_c/\partial\mu_l$) that is valid for both roots is:

$$\frac{\partial\mu_c}{\partial\mu_l} = E'_l \frac{1}{\sqrt{E'_c E_{cm} D^2}} .$$

NEE Energy and Jacobian



Inelastic NEE Solution Ranges

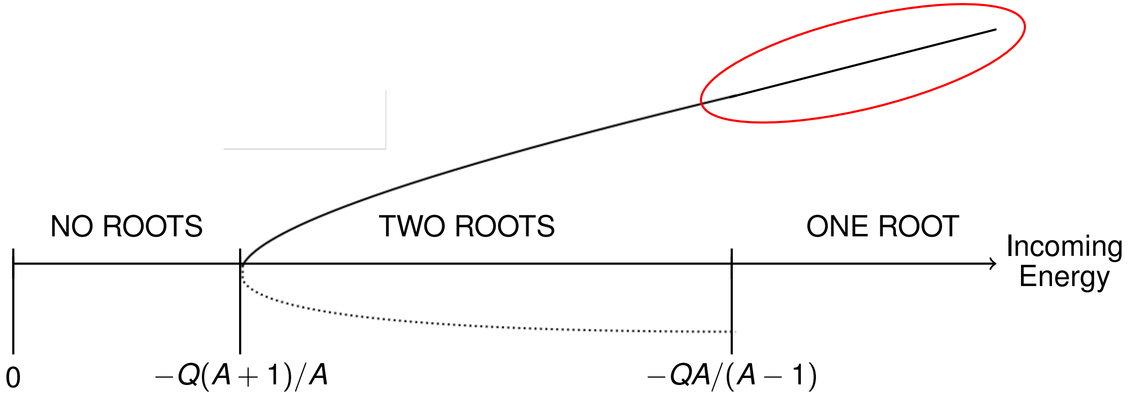


Two roots only valid for limited scattering angles: $\sqrt{1 - A^2 - QA(A+1)/E_I} < \mu_I < 1$

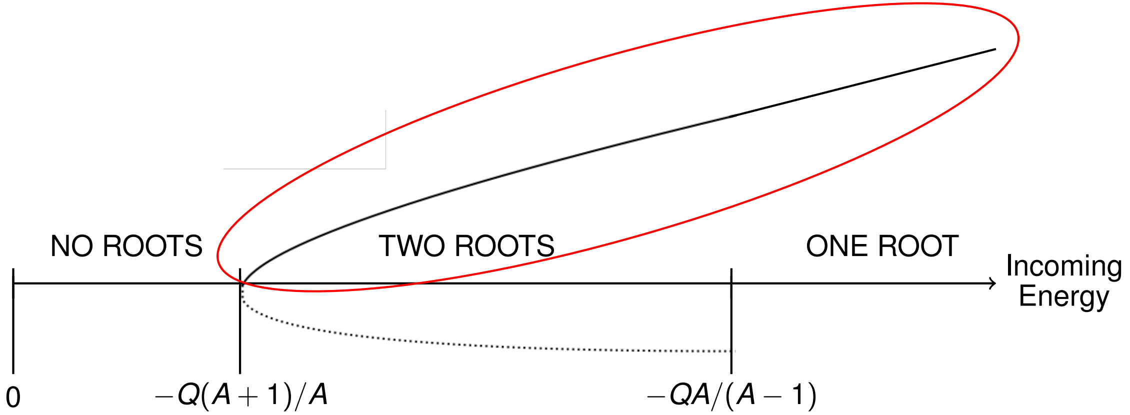
Examples of Two Root Ranges for Various Isotopes/Reactions

Isotope / Reaction	A	Q (MeV)	-Q(A+1)/A (MeV)	-QA/(A-1) (MeV)	ΔE
H-2 (n,2n)	1.9968	−2.2250	3.339	4.457	1.12 MeV
H-3 (n,2n)	2.9901	−6.2576	8.350	9.402	1.05 MeV
Li-6 (n,n'1)	5.9618	−1.5000	1.752	1.802	50.7 keV
Li-7 (n,n'1)	6.9557	−0.4776	0.546	0.5587	11.5 keV
Be-9 (n,2n)	8.9348	−1.5728	1.749	1.771	22.2 keV
B-11 (n,nα)	10.9147	−8.6637	9.457	9.538	80.1 keV
O-16 (n,n'1)	15.8575	−6.0494	6.431	6.457	25.7 keV
Al-26 (z,n') continuum	25.7637	−4.7240	4.907	4.915	7.40 keV
Fe-56 (n,n'1)	55.4544	−0.8468	0.862	0.862	280 eV
U-238 (n,n'1)	236.0058	−0.0449	0.045	0.045	0.810 eV

MCNP $\leq$ 6.3.0, NEE for Level Scattering



MCNP $\leq$ 6.3.0, NEE for Law 44 and Law 61



MCNP $\leq$ 6.3.0, Neutron NEE - Scattering Angle Issues

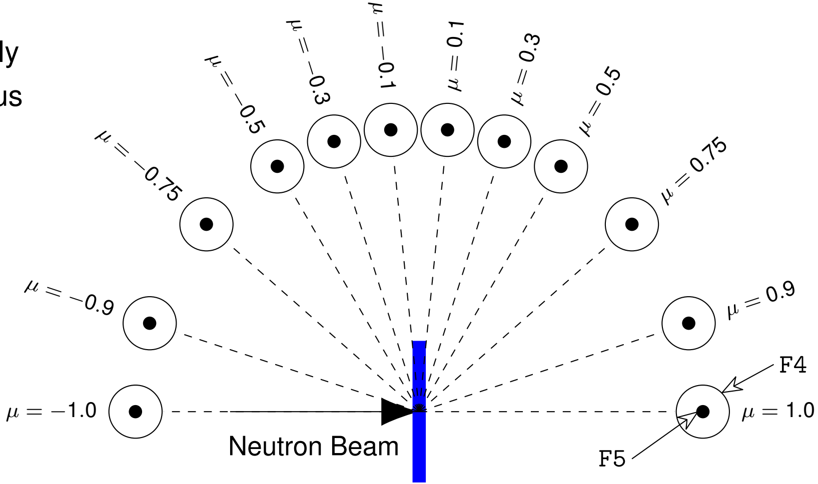
- Reactions are only possible if $-1.0 \leq \mu_c \leq 1.0$
- Floating point comparisons for $\mu_c \approx -1$ and $\mu_c \approx 1$ were not properly handled
  - some contributions were neglected
  - lead to minor underestimation
- Law 44 (Kalbach 87): Incorrect handling for $\mu_c < -1.0$ and $\mu_c > 1.0$
  - Was incorrectly reset to:
    $\mu_c = -1.0$ for $\mu_c < -1.0$,
    or
    $\mu_c = 1.0$ for $\mu_c > 1.0$
  - lead to overestimation, for backward scattering

MCNP $\geq$ 6.3.1, Corrections

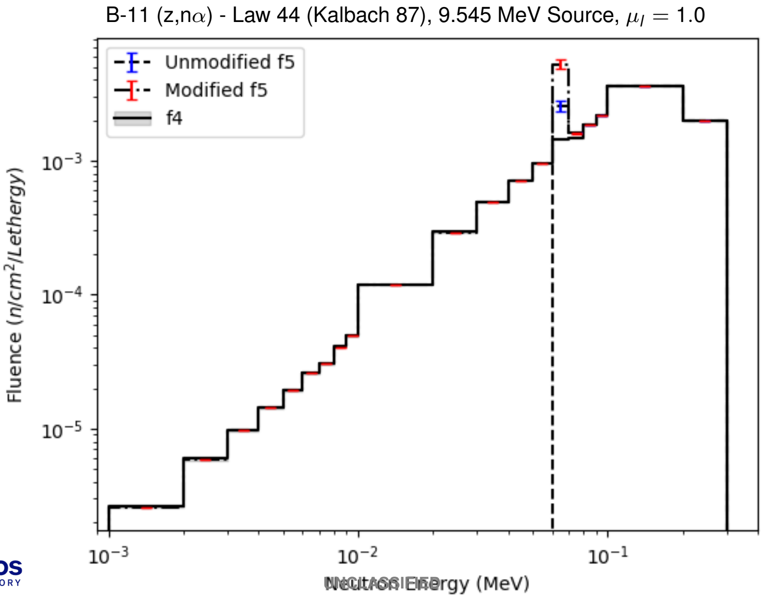
- All inelastic reactions implementations combined into a single implementation
- The correction solves for both roots [2].
- If $(-1.0 > \mu_c > -1.0 + \epsilon)$ then set $\mu_c = -1.0$
- If $(1.0 < \mu_c < 1.0 + \epsilon)$ then set $\mu_c = 1.0$

MCNP Tests with Single Reaction Cross-sections

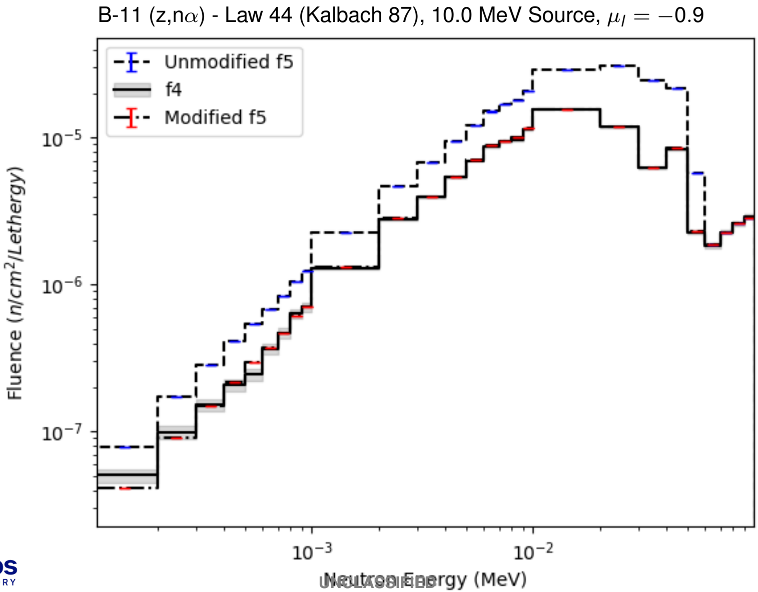
- Single reaction cross-sections generated with ACEtk
- Thin target
- Tally single scatter only
- Compare `F5` to `F4` torus



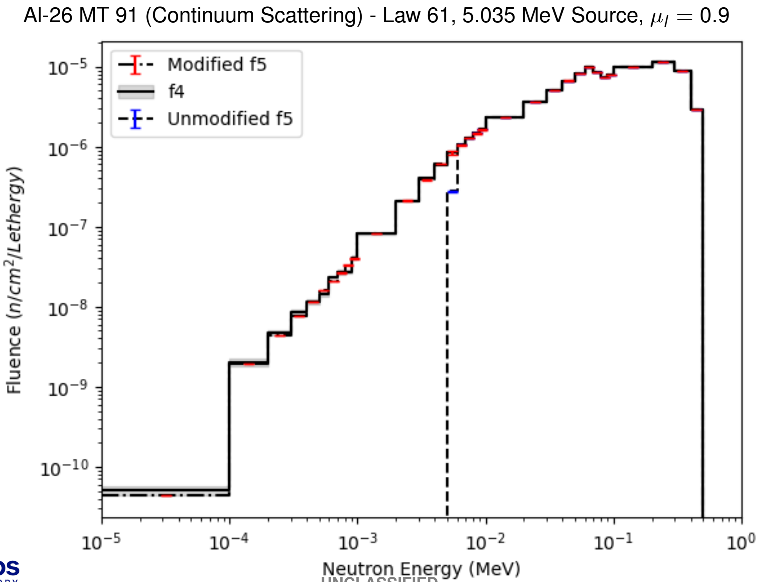
Testing - Law 44 (Kalbach 87) - Within Two Root Region



Law 44 (Kalbach 87) – Within Single Root Region

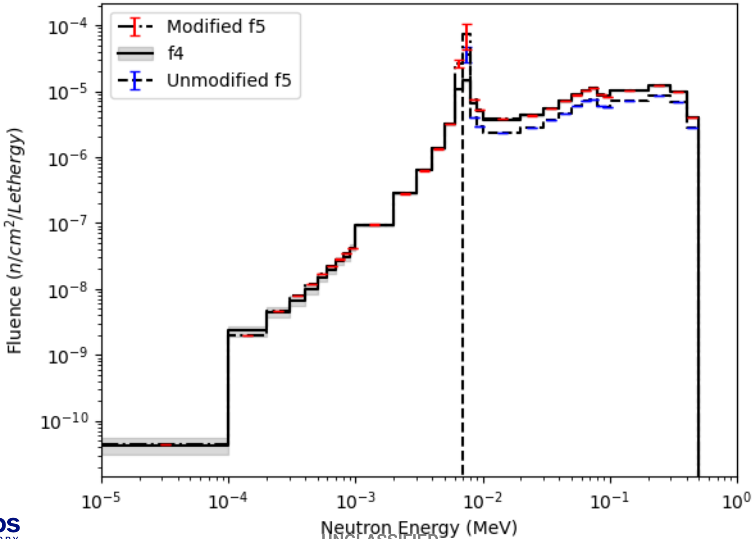


Law 61 (Tabulated Energy Angle) – Within Two Root Region



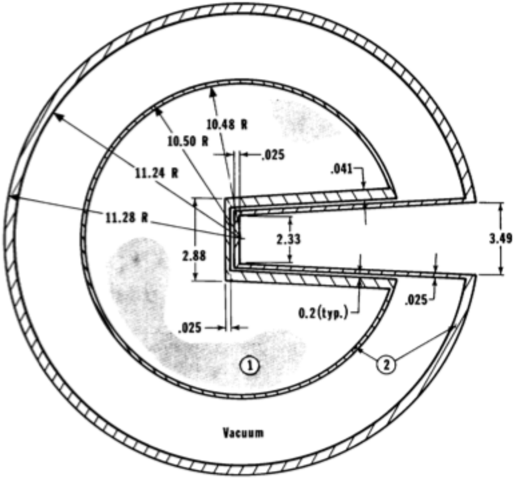
Law 61 (Tabulated Energy Angle) – Within Two Root Region

Al-26 MT 91 (Continuum Scattering) - Law 61, 5.035 MeV neutrons, $\mu_l = 1.0$

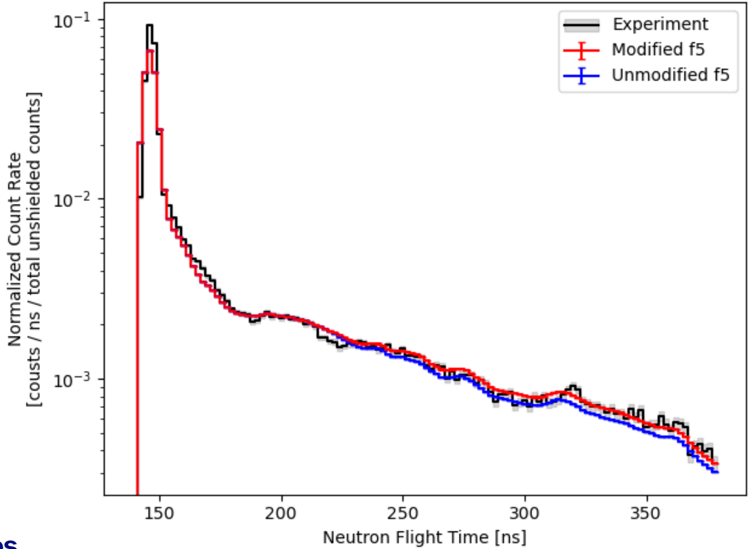


Integral Test - LLNL Pulse Sphere - D_2O Diagram

- D_2O sphere with fusion neutron generator
- Time-of-flight measurements



Integral Test - LLNL Pulse Sphere - D_2O Results



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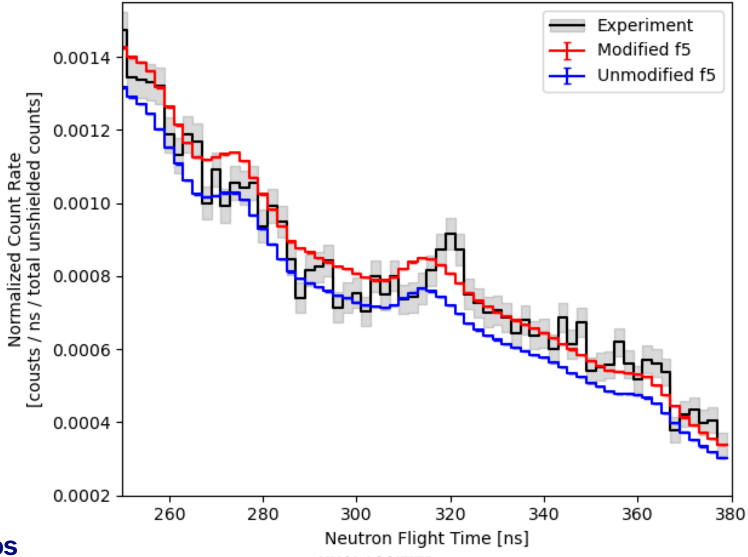

Questions

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