

# Multi-Step D1S: Restoring the Delayed Gammas Emitted Below the First Decay Step of an Open-Source D1S Implementation

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## 1. Introduction

The direct one-step (D1S) method obtains delayed-gamma quantities in a single coupled calculation, by replacing prompt gamma production with delayed-gamma production at the site of the activating neutron reaction [3]. A fully open-source D1S implementation has recently been released in OpenMC [2], constructing its delayed-gamma source from the nuclides produced directly by neutron reactions.

That construction is a single non-recursive pass over the reaction products of the collided nuclide, and the chain object it reads on the transport side represents no decay edge. Where the activation product itself decays to a gamma-emitting daughter, by a beta-minus branch or an isomeric transition, that emitter lies one step further down and no product is created for it. Its contribution to the emission rate is zero, and the emitter is absent from the transported population. The delayed gammas emitted below the first decay step are absent from the source term, so recovering them requires a calculation that carries the deeper terms in its source.

The identifier a delayed gamma carries is a scoring label: it is read only when the score is binned. One index suffices at the first decay step, since routes reaching one daughter share its decay constant and are correctly summed into one bin. What one index cannot separate is two chain depths, and the published implementation never has two, so widening it to the pair of emitting nuclide and chain step is a requirement of the extension and not the cause of the omission.

Fig. 1 shows the two halves of this. In (a) the source is built from the activation product, and the emitter one decay step below it is never created. In (b) the cobalt capture case, in which ground-state Co-60 is reached directly and again through the metastable state: the two routes carry different accumulated branching fractions, meaning the product of the branching fractions from the reaction down to that nuclide along each route, and a single-integer identifier folds them into one bin.

Decomposing the delayed-gamma source by chain step shows that the share at chain step 2 depends strongly on the activation path; the depth at which a truncation is placed therefore matters.

For MCNP-based D1S, multi-step decay chains were addressed by the novel one-step (N1S) method [1], which has not been implemented in OpenMC.

This work implements multi-step D1S: the decay chain below each activation product is carried further, every emitting member is given its own source term with the branching fractions accumulated down to it, and

every scoring event is tagged with its emitting nuclide and its chain step, so the two depths separate inside the tally. Exactly one emplaced emitter is selected probabilistically and banked at each collision.

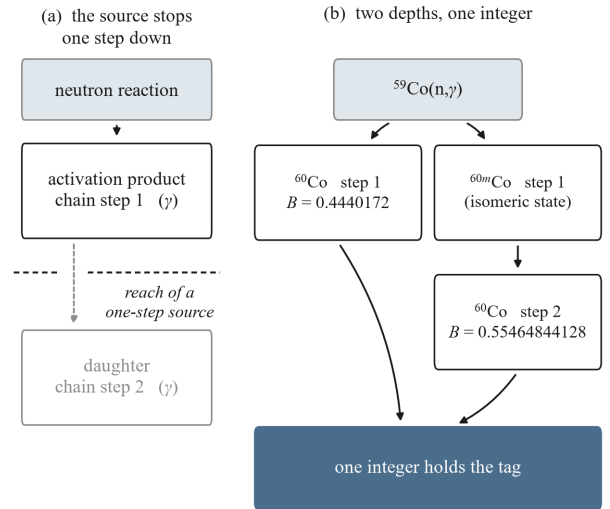


Fig. 1. Reach of a depth-1 delayed-gamma source (a), and the folded identifier in the cobalt capture case (b).

## 2. Method

### 2.1 The delayed-gamma source of an activation chain

A neutron reaction  $\rho$  on the collision nuclide produces a radioactive nuclide, which decays down a chain. A nuclide with more than one decay mode has more than one daughter, so the structure below the reaction is a rooted tree: the reaction's product is the root, and every other member is reached from the root by one succession of decays. Write  $v$  for a member of that tree,  $K_v$  for its nuclide,  $d_v$  for its depth with  $d_v = 1$  at the root, and  $u$  for the parent of  $v$ . Write  $\lambda_v$  for the total decay constant of  $K_v$  over all its decay modes,  $A_v$  for the number of atoms at  $v$  per activating reaction,  $b_{0,\rho}$  for the fraction of the reaction that produces the root of its tree, and  $b_{u \rightarrow v}$  for the fraction of the decays of  $u$  that produce  $v$ . The reaction is treated as instantaneous at  $t = 0$ , and the tree then evolves under decay alone,

$$\frac{dA_v}{dt} = \begin{cases} -\lambda_v A_v, & d_v = 1, \\ b_{u \rightarrow v} \lambda_u A_u - \lambda_v A_v, & d_v \geq 2, \end{cases}$$

$$A_v(0) = b_{0,\rho} \text{ at the root, } A_v(0) = 0 \text{ elsewhere. (1)}$$

Every member has one parent, so the equations of (1) along the path from the root to  $v$  form a linear cascade. Writing  $v_1, \dots, v_{d_v}$  for the members on that path in order, with  $v_{d_v} = v$ , and  $i$  and  $j$  for indices over them, the solution of the cascade separates into an accumulated fraction and a time density,

$$B_v = b_{0,\rho} \prod_{i=2}^{d_v} b_{v_{i-1} \rightarrow v_i} \quad (2)$$

$$P_v(t) = \sum_{i=1}^{d_v} \left( \prod_{\substack{j=1 \\ j \neq i}}^{d_v} \frac{\lambda_{v_j}}{\lambda_{v_j} - \lambda_{v_i}} \right) \lambda_{v_i} e^{-\lambda_{v_i} t} \quad (3)$$

$$\lambda_v A_v(t) = B_v P_v(t) \quad (4)$$

Equation (3) holds where the decay constants along a path are distinct and strictly positive, each being the total decay constant of its nuclide.  $B_v$  is the accumulated fraction of the reaction that reaches  $v$ , the product of the branching fractions from the reaction down to  $v$ , and the branching fractions are carried by that fraction alone.  $P_v$  is the activity of (4) divided by that accumulated fraction: the probability density of the time from the reaction to a decay at  $v$ , conditional on the decays following the path to  $v$ , being the density of the sum of the  $d_v$  independent exponential lifetimes along that path, so it integrates to unity over all cooling times. A finite irradiation replaces  $P_v$  by its convolution with the irradiation history.

Every member that emits gammas contributes to the delayed-gamma source in proportion to its activity. Writing  $M_K$  for the gammas emitted per decay of nuclide  $K$ , a property of the nuclide, and  $\mathcal{V}$  for the set of members the method carries, the delayed-gamma emission rate of one tree, per activating reaction, is

$$S(t) = \sum_{v \in \mathcal{V}} B_v P_v(t) M_{K_v} \quad (5)$$

The two methods differ in the set  $\mathcal{V}$  retained in this sum. Conventional D1S builds its source from the nuclides the reaction produces directly, so  $\mathcal{V}$  holds the roots alone and (5) reduces to its  $d_v = 1$  term, with  $B_v = b_{0,\rho}$  and  $P_v(t) = \lambda_v e^{-\lambda_v t}$ , the ordinary single-nuclide decay factor. Multi-step D1S carries the same sum to the emitting members below the first, keeping one member per nuclide within each tree, down to a bounded depth; the chains examined here lie well within that bound. A member with  $M_{K_v} = 0$  passes the tree to the members below it, so an emitter standing behind it is reached.

Throughout this work a gamma is filed by the nuclide whose decay produces it, so chain step 1 holds the gammas emitted in the decay of the reaction's direct product; such a gamma is strictly a de-excitation line of the daughter nuclide, and the tag files it under the decaying nuclide.

Integrating (5) over all cooling times leaves the number of gammas the carried members emit, per activating reaction,

$$\int_0^\infty S(t) dt = \sum_{v \in \mathcal{V}} B_v M_{K_v} \quad (6)$$

which is free of the cooling time and is the quantity the transport calculation produces.

## 2.2 Realisation of the multi-step source in the transport calculation

D1S realises a source term of this kind by producing the delayed gamma at the site of the activating reaction rather than in a separate transport step, carrying the decay information on the particle. Each carried member of (5) is produced at the rate of the reaction that produces it, multiplied by its yield,

$$y_v = B_v M_{K_v} \quad (7)$$

which is the term of  $v$  in (6), the gammas that member emits over all time per activating reaction.

The transport calculation realises this at the collisions themselves. The yields are combined with the cross sections of the producing reactions once; at each collision one delayed gamma is banked, its weight the incident neutron weight scaled by the ratio of that combined cross section to the total cross section, and its member drawn in proportion to its own contribution:

$$w_\gamma = w \frac{\sum_{v \in \mathcal{V}} y_v \sigma_{\rho(v)}(E)}{\sigma_{\text{tot}}(E)} \quad (8)$$

$$p_v = \frac{y_v \sigma_{\rho(v)}(E)}{\sum_{v' \in \mathcal{V}} y_{v'} \sigma_{\rho(v')}(E)} \quad (9)$$

with  $w$  the weight of the incident neutron,  $w_\gamma$  that of the banked gamma,  $E$  the incident neutron energy,  $\rho(v)$  the reaction whose tree contains  $v$ ,  $\sigma_{\rho(v)}$  its cross section, and  $\sigma_{\text{tot}}$  the total cross section of the collision nuclide; the sums run over the carried members of every reaction of that nuclide, the same set that (5) and (6) sum over. Both expressions are quotients of cross sections at one energy, so both can be evaluated at the collision. Weighting each collision by (8) and drawing the member by (9) banks, per source neutron, each carried member's yield multiplied by the number of its producing reactions per source neutron; summing a cross-section quotient of this kind over the collisions is the collision estimator of a reaction rate, which is the cross section integrated against the neutron flux. The gammas per decay  $M_K$  is carried on the statistical weight rather than on the particle count, so one transported gamma stands for the multiplicity of its member. Its energy is sampled from the line spectrum of its emitting nuclide, so that spectrum governs how far the gamma travels and what it contributes to a track-length tally; the spectrum is absent from the equations above because none of them needs it, and not because the tallied quantities are independent of it.

Because the terms of (5) must stay separable after transport, each banked gamma carries the pair of its emitting nuclide and its chain step  $n$ , the depth of the member it was drawn from. The identifier is written once when the gamma is banked, is carried through the

secondary particle bank and through transport unaltered, and is read at scoring by filters on emitting nuclide and on chain step, each filter binning every event by its tag, so the terms of (5) score into separate bins of one joint tally. Fig. 2 shows the chain, the terms each method carries, and the tally they are scored into.

The reported quantity is the gamma track length accumulated inside the tallied cell per source neutron, restricted to one pair of tags,

$$\Phi_{K,n} = \frac{1}{H} \sum_{g \in (K,n)} w_g \ell_g, \quad (10)$$

with  $K$  and  $n$  the emitting-nuclide and chain-step tags,  $H$  the number of source neutrons simulated,  $g$  running over the scoring segments made in the tallied cell by the gammas of that bin, and  $\ell_g$  the track length of segment  $g$ . Every bin is scored in one and the same cell. The division by  $H$  is the whole of the normalisation, so  $\Phi_{K,n}$  is a track length per source neutron, and the cell volume, being common to every bin, cancels from every share and ratio reported here. The cooling-time dependence is restored afterwards by weighting each bin with the time density of the member that feeds it,

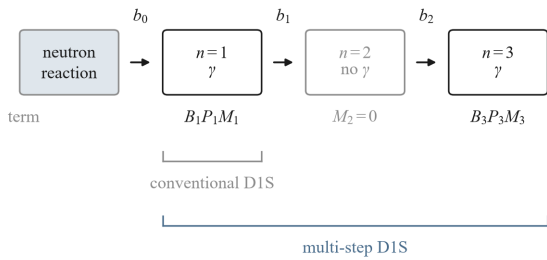
$$\Phi_{K,n}(t) = P_v(t) \Phi_{K,n} \quad (11)$$

and every value reported in this work is the tally as accumulated during transport, before any cooling-time factor is applied to it.

The comparison across cases uses the share of that quantity lying at chain step 2,

$$f_2 = \frac{\sum_K \Phi_{K,2}}{\sum_K \sum_n \Phi_{K,n}}. \quad (12)$$

(a) the source is a sum over the members of the chain



(b) the joint tally

|                        | chain step $n$ |          |   |                             |
|------------------------|----------------|----------|---|-----------------------------|
|                        | 1              | 2        | 3 |                             |
| emitting nuclide $K_1$ | $\gamma$       |          |   | each term keeps its own bin |
| emitting nuclide $K_2$ |                | $\gamma$ |   |                             |

Fig. 2. The activation chain and the terms each method carries (a), and the joint (emitting nuclide  $\times$  chain step) tally they are scored into (b).

## 2.3 Relation to NIS

NIS reaches multi-step chains by decomposing the decay chain below an activation product into linear routes, and banking the gammas of every member of every route [1]. In the notation of Section 2.1, a route to an emitting nuclide is the path to a member of the tree carrying that nuclide, so NIS carries every such member, each with its own accumulated fraction and time density, while multi-step D1S keeps one of them per nuclide within each tree, written  $v^*$ . For that nuclide in that tree,

$$\sum_{v: K_v=K} B_v P_v(t) \geq B_{v^*} P_{v^*}(t) \quad (13)$$

the sum running over the members of the tree carrying  $K$ .

Where an emitting nuclide is reached by more than one route, NIS sums them all and multi-step D1S retains one, so the source of equation (5) is smaller by the terms of the remaining routes.

The two also differ in what they bank. NIS banks a number of gammas per activating collision that the chain below the activation product determines, while multi-step D1S banks one at every depth. Carrying  $M_K$  on the statistical weight rather than on the particle count is what lets one banked gamma stand for the whole multiplicity, so the two carry the same expected track length on the terms they share. The secondary population NIS transports therefore grows with that chain, while the population multi-step D1S transports is set by the number of collisions alone, so carrying the sum deeper leaves its transport cost unchanged.

## 3. Results

### 3.1 Cases considered and calculation conditions

Five activation paths were considered, chosen to span the mechanisms by which the chain member below the first is populated or left empty. C1 activates natural zirconium through  $\text{Zr-94}(n,\gamma)$  to  $\text{Zr-95}$ . C2 activates  $\text{Mo-98}$  through  $(n,\gamma)$  to  $\text{Mo-99}$ , whose beta-minus decay reaches  $\text{Tc-99m}$  and  $\text{Tc-99}$ . C3 activates  $\text{Ag-109}$  through  $(n,\gamma)$  to  $\text{Ag-110m}$ , below which the chain reaches a stable terminus. C4 activates  $\text{Ni-58}$  through the threshold reaction  $(n,2n)$  to  $\text{Ni-57}$ , whose electron-capture decay reaches  $\text{Co-57}$ . C5 activates  $\text{Co-59}$  through  $(n,\gamma)$  to both the ground state of  $\text{Co-60}$  and its metastable state, which reaches the ground state by isomeric transition, so  $\text{Co-60}$  emits at two chain steps. Each tally declares the emitters named for its case, C1 declaring the chain head alone.

The targets are natural zirconium at  $6.51 \text{ g/cm}^3$ , of atom fractions  $\text{Zr-90}$  0.5145,  $\text{Zr-91}$  0.1122,  $\text{Zr-92}$  0.1715,  $\text{Zr-94}$  0.1738 and  $\text{Zr-96}$  0.0280, and the separated nuclides  $\text{Mo-98}$  at 10.28,  $\text{Ag-109}$  at 10.49,  $\text{Ni-58}$  at 8.91 and  $\text{Co-59}$  at  $8.90 \text{ g/cm}^3$ .

The calculations were run with OpenMC 0.15.3, extended as described in Section 2.2, with decay and

transmutation data from an ENDF/B-VIII.1-based evaluation [4].

Table I: Conditions common to all five cases.

| Quantity                     | Value                                                         |
|------------------------------|---------------------------------------------------------------|
| Geometry                     | sphere, R = 10 cm                                             |
| Boundary                     | reflective                                                    |
| Source                       | point at the origin, isotropic, 14 MeV monoenergetic neutrons |
| Total histories              | 1E8                                                           |
| Neutron and gamma data       | ENDF/B-VIII.1, continuous energy                              |
| Decay and transmutation data | ENDF/B-VIII.1 depletion chain (fast)                          |

### 3.2 Verification of the implementation

Each of the five calculations produces one tally binned jointly by emitting nuclide and chain step, given in Table II. C4 and C5 admit a direct check of it against the chain — the first on which bins receive events, the second on the magnitude they receive.

Table II: Volume integrated delayed-gamma flux (Units: cm)

| Case | Emitting nuclide | Step 1 — carried by conventional D1S | Step 2 — added by multi-step D1S     | Step 3 | $f_2$ (%) |
|------|------------------|--------------------------------------|--------------------------------------|--------|-----------|
| C1   | Zr-95            | $9.708\text{E-}1 \pm 1.02\text{E-}4$ | 0                                    | 0      | 0         |
| C2   | Mo-99            | $1.427\text{E}0 \pm 1.45\text{E-}4$  | 0                                    |        | 24.27     |
|      | Tc-99m           | 0                                    | $4.575\text{E-}1 \pm 3.65\text{E-}5$ |        |           |
|      | Tc-99            | 0                                    | 0                                    |        |           |
| C3   | Ag-110m          | $8.820\text{E-}1 \pm 7.30\text{E-}5$ | 0                                    |        | 0         |
| C4   | Ni-57            | $1.379\text{E-}1 \pm 5.24\text{E-}5$ | 0                                    |        | 5.48      |
|      | Co-57            | 0                                    | $7.991\text{E-}3 \pm 5.08\text{E-}6$ |        |           |
| C5   | Co-60m           | $1.536\text{E-}2 \pm 1.52\text{E-}5$ | 0                                    |        | 55.50     |
|      | Co-60            | $8.439\text{E}0 \pm 7.72\text{E-}4$  | $1.054\text{E}1 \pm 9.91\text{E-}4$  |        |           |

In C4 the chain Ni-58(n,2n) to Ni-57 to Co-57 places Ni-57 at chain step 1 and Co-57 at chain step 2, so the pairs (Ni-57, step 2) and (Co-57, step 1) fall outside the terms of equation (5). Both are exactly zero in Table II, in the flux and in its standard deviation alike, while (Co-57, step 2) is strictly positive in both. A zero of that kind arises only where no scoring event occurred in any history, so those two bins are structurally empty.

In C5 ground-state Co-60 is reached directly and again through the metastable state, so one emitting nuclide occupies two chain steps. The two are the two activation products of that reaction, each the root of a tree of its own, and retention applies within each tree separately, so both bins are carried. Writing  $v$  and  $v'$  for the two members and  $\mathbb{E}[\cdot]$  for the expectation over the simulation, the two bins stand in the ratio

$$\frac{\mathbb{E}[\Phi_{K,n}]}{\mathbb{E}[\Phi_{K,n'}]} = \frac{B_v}{B_{v'}} \quad (14)$$

which holds where the two bins carry the same nuclide at different chain steps and their trees are started by the same reaction, as they are here. The step-2 bin is fed by the route through the metastable state and the step-1 bin by the direct route, and their ratio in Table II is 1.2492. The depletion chain [4] gives Co-59(n, $\gamma$ ) a branching fraction of 0.44402 to ground-state Co-60 and 0.55598 to the metastable state, and gives the metastable state an isomeric-transition branch of 0.9976 to the ground state. Equation (2) accumulates these along each route: 0.44402 for the direct route, and 0.55465, the product of the other two, for the route through the metastable state. The analytic solution of the chain equation puts the two bins in that ratio, and the multi-step D1S tally reproduces it to five significant figures, the difference lying within the statistical uncertainty of the tally. Both sides use the same branching fractions, so the agreement demonstrates that  $B_v$  accumulates along a two-step chain and that the tag survives the secondary bank and transport.

### 3.3 Contribution of the second chain step

The share  $f_2$  of equation (12) was formed from the joint tally of each case and is given in the last column of Table II. It is 0, 24.27, 0, 5.48 and 55.50 % for C1 to C5. C1 declares only the chain head to its tally and C3 reaches a stable terminus below the first step, so both shares are structurally zero. The three positive shares follow the decay of the activation product — Tc-99m across a beta-minus decay in C2, Co-57 across an electron-capture decay in C4, and ground-state Co-60 across an isomeric transition in C5. In C5 the two Co-60 bins carry one nuclide at two chain steps, so their ratio is the same in dose as in flux.

## 4. Conclusions and Future Study

1. The delayed-gamma source of the published open-source D1S implementation is the first term alone of the sum over the activation chain, so recovering the gammas emitted below the first decay step requires a calculation that carries the deeper terms.

2. Multi-step D1S was implemented, carrying the sum to the emitting members below the first with the branching fractions accumulated down to each, and tagging every scoring event by emitting nuclide and chain step. In the nickel case the two cross bins of one joint tally are exactly zero in both the flux and its standard deviation, and in the cobalt case the ratio of the two chain-step bins of ground-state Co-60 agrees to five significant figures with the 1.2492 that equation (2) gives from the branching fractions of the decay data.

3. The share of the scored gamma flux at chain step 2 runs from 0 to 55.50 % with the activation path, the largest in the cobalt case, so the depth at which the sum is truncated matters; the two zeros are structural, for the two distinct reasons given in Section 3.3.

For the future study, a dose-response score will be added to the same joint tally, carrying the decomposition

from flux into dose, with the share at each chain step set by the dose response of its emitting nuclide's spectrum.

### **Acknowledgments**

This work was supported by the National Research Foundation of Korea (NRF) funded by the Korean government (MSIT) (RS-2026-25545634).

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