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From Sparse Measurements to Dense DDX: Bayesian Tensor Modeling of Proton-^{nat}Pb for ADS Source Terms

Authors: LIU, Miss Huizi, HUANG, Mr. Yingge, Su, Dr. Jun, WANG, Miss Hui, XIAO, Mr. Erxi, HUANG, Jiali, FENG, Yujie, GU, Mr. Fuchang, CHEN, Qiafeng, Su, Dr. Jun

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Abstract

Accurate spallation-neutron source terms are essential for accelerator-driven systems (ADS), yet double-differential cross-section (DDX) measurements remain sparse—particularly for proton-^{nat}Pb, a canonical ADS target. We present a data-driven pathway from sparse measurements to dense DDX using a Bayesian tensor model together with a physics-consistent interpolation scheme tailored for ADS source-term generation. A total of 1{,}727 DDX points for proton-^{nat}Pb, compiled from EXFOR and literature, spanning eight incident energies ($10_{\text{MeV-3}}$GeV) and seven angles (7.5°-150°), are used in full to fit the tensor model. Under the optimal configuration, the model shows strong in-sample reproduction on a log scale: 96.3% of points lie within ±20% of experiment, 80.6% within ±10%, and 52.46% within ±5%. For out-of-measurement checks, we compare predictions with the Bertini intranuclear-cascade model in Geant4 (and BERT_HP where available) on common discrete grids: agreement is close below 10~MeV; in the 20-100~MeV band, where BERT/BERT_HP are known to underestimate data, our predictions remain physically plausible. To deliver application-ready inputs, we construct a high-resolution database via bilinear interpolation in (E_p, θ) on self-similar energy slices $\kappa = \ln(E_n/E_p)$ (default $\Delta\kappa = 0.2$), evaluated on a regular grid with 1~MeV spacing in E_p and 0.5° in θ, with a no-extrapolation policy. The interpolants preserve evaporation-like low-energy behavior and forward-peaked high-energy emission and are consistent with Geant4 trends. The resulting proton-^{nat}Pb DDX database, covering the CiADS design point (500~MeV) and its neighborhood, is ready to be coupled to transport codes (e.g., OpenMC) for anisotropic source-term calculations and can be extended to other targets and reactions.

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Preamble

From Sparse Measurements to Dense DDX: Bayesian Tensor Modeling of Proton-natPb for ADS Source Terms

Huizi Liu,[1] Yingge Huang,[1] Hui Wang,[1] Erxi Xiao,[1] Jiali Huang,[1] Yujie Feng,[1] Fuchang Gu,[1] Qiafeng Chen,[1] and Jun Su[1],†
[1]Sino-French Institute of Nuclear Engineering and Technology, Sun Yat-sen University, Zhuhai 519082, China

Accurate spallation-neutron source terms are essential for accelerator-driven systems (ADS), yet double-differential cross-section (DDX) measurements remain sparse—particularly for proton-natPb, a canonical ADS target. We present a data-driven pathway from sparse measurements to dense DDX using a Bayesian tensor model together with a physics-consistent interpolation scheme tailored for ADS source-term generation. A total of 1,727 DDX points for proton-natPb, compiled from EXFOR and literature, spanning eight incident energies (10 MeV-3 GeV) and seven angles (7.5°-150°), are used in full to fit the tensor model. Under the optimal configuration, the model shows strong in-sample reproduction on a log scale. For out-of-measurement checks, we compare predictions with the Bertini intranuclear-cascade model in Geant4 (and BERT HP where available) on common discrete grids: agreement is close below 10 MeV; in the 20-100 MeV band, where BERT/BERT HP are known to underestimate data, our predictions remain physically plausible. To deliver application-ready inputs, we construct a high-resolution database via bilinear interpolation in (Ep,) on self-similar energy slices = ln(En/Ep), evaluated on a regular grid with 1 MeV spacing in Ep and 0.5° in , with a no-extrapolation policy. The interpolants preserve evaporation-like low-energy behavior and forward-peaked high-energy emission and are consistent with Geant4 trends. The resulting proton-natPb DDX database, covering the CiADS design point (500 MeV) and its neighborhood, is ready to be coupled to transport codes (e.g., OpenMC) for anisotropic source-term calculations and can be extended to other targets and reactions.

Keywords: Spallation neutrons; Double-differential cross sections (DDX); Bayesian tensor model; Proton-natPb; ADS source terms

Introduction

Nuclear energy offers notable advantages, including high energy density and stable operational performance; however, the management of long-lived high-level radioactive waste remains a major challenge [1]. The accelerator-driven system (ADS) has emerged as a promising route by enabling the transmutation of long-lived radionuclides into short-lived or stable isotopes, thus reducing both radioactivity and volume [2, 3]. Compared with conventional critical reactors, ADS can exhibit favorable neutron economy and transmutation performance in appropriate designs [4].

ADS utilizes high-energy protons to bombard a spallation target, generating fast neutrons that drive the subcritical core to sustain transmutation reactions [5]. Consequently, the accuracy of the external neutron source term is of critical importance. Extensive studies have demonstrated that the neutron source term significantly influences both the computational accuracy and operational performance of the ADS reactor. For instance, Jiang Xiao-feng et al. [6] employed the ANIAN-DOT4.2-ORIGEN2 code to analyze the IAEA ADS benchmark problem and concluded that the external neutron intensity must be dynamically adjusted in synchronization with fuel burnup to maintain the reactor’ s rated power output. Similarly, Cao Jian et al. [7] utilized the MCNP code to calculate transmutation reaction rates for nine types of minor actinides (MA) and long-lived fission products (LLFP), revealing that higher external neutron energies lead to increased transmutation rates across all nuclides. Furthermore, Pan Dong-mei et al. [8] conducted neutron physics simulations of multi-region ADS cores using the VisualBUS4.2 code and found that both the number and spatial configuration of external neutron sources markedly affect the effective multiplication factor (keff) and the core’s power distribution. Collectively, these findings underscore that the precision of the neutron source term is fundamentally linked to key reactor characteristics, including core neutronics behavior, power regulation, and safety evaluation.

In practice, source terms in target–core coupling simulations are often simplified. For example, the OECD/NEA ADS benchmark adopts ring-shaped volume sources, a broad HETC-based spectrum, and isotropic emission [9]; the optimization design of an ADS transmutation reactor sometimes uses Maxwellian fission spectra with isotropy [10]. Such approximations introduce two uncertainties. First, the fission neutron spectrum differs substantially from the actual energy distribution of spallation neutrons; spallation reactions can generate high-energy neutrons with energies approaching that of the incident protons [11]. Second, spallation neutrons exhibit pronounced forward-peaked angular distribution, with high-energy neutron yield decreasing significantly as the emission angle increases [12]. Zhao Zijia et al. [13] further demonstrated in their neutron physics analysis of an ADS spallation target that the assumption of isotropy underestimates the contribution of forward-directed neutrons, thereby affecting predictions of keff and core power distribution. Therefore, fission-spectrum and isotropic assumptions can lead to biased results and are not fully justified for accurate source modeling.

A key reason for these approximations is the scarcity of double-differential cross-section (DDX) measurements for spallation neutrons. Although EXFOR includes DDX for proton-induced spallation on about 14 target materials (from light to heavy nuclei) at incident energies between 63 MeV and 3 GeV and angles between 7.5° and 160°, the coverage is incomplete and lacks systematic consistency [14]. In particular, for natural lead, which is a key ADS target material, available measurements exist only at a few discrete Ep and values [15–

18]. Major evaluated libraries (ENDF/B, JENDL, JEFF) provide only partial isotope-specific data at select energies (e.g., 150, 200, 1000, 3000 MeV), without a comprehensive evaluation for natural lead. Given that the China Initiative ADS (CiADS) plans a 500 MeV, 5 mA superconducting linac [19], filling these data gaps is important for design and optimization.

Parallel to data efforts, spallation models have been benchmarked extensively. In 2008, the International Atomic Energy Agency (IAEA) launched the Global Spallation Model Benchmark that compared 17 mainstream models (CEM, INCL++, Geant4-Bertini, PHITS, etc.) [20, 21]. Despite progress, limitations persist: below 100 MeV, many models struggle in the 20–100 MeV neutron range and in forward-angle high-energy emissions [22, 23]. David et al. [24] recommended extending the applicability of spallation reaction models to the 10–15 GeV energy range and incorporating additional physical degrees of freedom to improve their fidelity. Subsequent experiments revealed model-specific deficiencies and database inconsistencies. In 2023, Iwamoto et al. [17] measured the DDX of neutrons from 103 MeV protons impinging on natPb and 209Bi targets, revealing specific deficiencies in models, as well as in existing nuclear databases. Sun Qi et al. [25], motivated by the design requirements of the CiADS project, employed GEANT4 and FLUKA frameworks to compute neutron DDX for 256 MeV protons incident on various target materials. These results motivate higher-fidelity approaches to complement existing models and data.

Recently, machine learning has shown promise in nuclear data, spanning charge radii, masses, fission cross sections, fragmentation, the EoS, and data evaluation/prediction [26–38]. Within this context, our group have adapted the Bayesian Gaussian CP (BGCP) tensor model to neutron-induced fission product yields [40, 41], (n,2n) cross sections of LLFPs [42] and elastic proton-scattering differential cross sections [43], providing a foundation to extend tensor-based modeling to spallation-neutron DDX. This work is part of a broader project to build a high-energy nucleon–nucleus database for CiADS reactor analysis. The DDX of neutrons from proton–natPb reactions constitutes a necessary subset for source-term construction. In this study, we focus on proton-induced spallation on natural lead. Using the tensor model, we predict and reconstruct DDX across eight incident energies (10 MeV–3 GeV) and seven scattering angles (7.5°–150°), based on 1,727 experimental points from EXFOR and literature [15–18]. To provide application-ready inputs, we further construct a high-resolution database by performing interpolation in (Ep,) on fixed self-similar energy slices = ln(En/Ep). For external checks where measurements are absent, we compare with BERT as implemented in Geant4 (and BERT HP where available), using a common binning and the same DDX conversion from counts.

Theoretical Framework

A. Tensor Model

We adopt a Bayesian Gaussian CP (BGCP) tensor model to complete and predict multiway nuclear data with missing entries. BGCP combines CANDECOMP/PARAFAC (CP) decomposition with Bayesian inference, enabling robust imputation under sparsity while explicitly quantifying predictive uncertainty.

a. Tensorization of DDX data. The DDX for spallation neutrons produced by proton-induced reactions on natural lead depends on three independent variables: incident proton energy, scattering angle, and outgoing neutron energy. To reduce scale variation across energy decades, the outgoing neutron energy is logarithmically transformed before binning. The resulting data are arranged into a third-order tensor $\mathcal{S} \in \mathbb{R}^{I \times J \times K}$, where the element σ_{ijk} corresponds to incident energy bin $E_{p,i}$, angle bin θ_j, and outgoing neutron-energy bin $E_{n,k}$. Measured entries from EXFOR and the literature provide a subset of observations indexed by the set $\Omega = \{(i, j, k, p)\}$, where p enumerates replicate measurements (e.g., different experiments) for the same (i, j, k).

b. CP factorization. Let L be the CP rank and $\mathbf{Z} \in \mathbb{R}^{I \times L}$, $\mathbf{D} \in \mathbb{R}^{J \times L}$, $\mathbf{E} \in \mathbb{R}^{K \times L}$ be the factor matrices. The reconstructed tensor is $\hat{\mathcal{S}} = \sum_{l=1}^{L} \mathbf{z}_{:l} \circ \mathbf{d}_{:l} \circ \mathbf{e}_{:l}$, so that the model mean for an entry is $\hat{\sigma}_{ijk} = \sum_{l=1}^{L} z_{il} d_{jl} e_{kl}$. Here "$\circ$" denotes the outer product.

c. Likelihood. For each observed replicate $(i, j, k, p) \in \Omega$, we assume a Gaussian noise model $\sigma_{ijk}^{(p)} \sim \mathcal{N}(\hat{\sigma}_{ijk}, \tau_\epsilon^{-1})$, where $\mathcal{N}(\cdot)$ denotes a Gaussian distribution, τ_ϵ is the observation precision. If reported experimental uncertainties are available, the model can use entry-specific precisions $\tau_{ijk}^{(p)}$ in place of a global τ_ϵ.

d. Priors. Rows of the factor matrices are given independent Gaussian priors with shared hyperparameters $\mathbf{z}_i \sim \mathcal{N}(\mu^{(z)}, (\Lambda^{(z)})^{-1})$, $\mathbf{d}_j \sim \mathcal{N}(\mu^{(d)}, (\Lambda^{(d)})^{-1})$, $\mathbf{e}_k \sim \mathcal{N}(\mu^{(e)}, (\Lambda^{(e)})^{-1})$, where each $\Lambda^{(\cdot)}$ is a precision matrix. Conjugate Gamma priors are placed on the precisions, $\tau_\epsilon \sim \Gamma(a_0, b_0)$, and Normal-Wishart hyperpriors may be used for $(\mu^{(\cdot)}, \Lambda^{(\cdot)})$.

e. Gibbs sampling. Thanks to conjugacy, the full conditionals are Gaussian or Gamma in closed form. For example, conditioning on $\mathbf{D}$, $\mathbf{E}$, τ_ϵ, the posterior for $\mathbf{z}_i$ is

$$\hat{\Lambda}_i^{(z)} = \Lambda^{(z)} + \tau_\epsilon \sum_{(j,k,p)} \mathbb{I}_{ijkp} (\mathbf{d}_j \odot \mathbf{e}_k)(\mathbf{d}_j \odot \mathbf{e}_k)^\top,$$

$$\hat{\mu}_i^{(z)} = \left(\hat{\Lambda}_i^{(z)}\right)^{-1} \left[\Lambda^{(z)} \mu^{(z)} + \tau_\epsilon \sum_{(j,k,p)} \mathbb{I}_{ijkp} (\mathbf{d}_j \odot \mathbf{e}_k) \sigma_{ijk}^{(p)} \right].$$

Here "$\odot$" is the Hadamard product, $\mathbb{I}_{ijkp}$ is 1 for index (i, j, k, p) with measurement and 0 for the case without measurement. Analogous expressions hold for $\mathbf{d}_j$ and $\mathbf{e}_k$ by cycling the tensor modes. Similarly, using the likelihood with the Gaussian form and the prior term of τ_ϵ with the Gamma form, it will give the posterior with the Gamma distribution. Let $N_{\text{obs}} = \sum \mathbb{I}[(i,j,k,p) \in \Omega]$. The conditional posterior of τ_ϵ is

$$\tau_\epsilon \mid \cdots \sim \Gamma\left(a_0 + \frac{1}{2}N_{\text{obs}},\ b_0 + \frac{1}{2}\sum_{(i,j,k,p)}\left(\sigma_{ijk}^{(p)} - \widehat{\sigma}_{ijk}\right)^2\right).$$

We alternate sampling of $\mathbf{Z}$, $\mathbf{D}$, $\mathbf{E}$, τ_ϵ; after burn-in, posterior means (or medians) of $\widehat{\sigma}_{ijk}$ are reported together with credible intervals.

Implementation notes. We provide the bin definitions for (E_p, θ, E_n), the CP rank L selection procedure, prior hyperparameters, number of chains/iterations/burn-in, random seeds, and units (e.g. mb $\text{sr}^{-1}\text{MeV}^{-1}$) to ensure full reproducibility.

B. Interpolation Method

The tensor model provides discrete DDX values σ_{ijk} on a grid indexed by i (incident proton energy $E_{p,i}$), j (scattering angle θ_j), and k (outgoing neutron energy sampled on the log grid $\xi_k = \ln E_{n,k}$). For applications requiring continuous queries, we construct a three-dimensional linear interpolation scheme with an energy-axis reparametrization that respects the kinematic scaling.

a. Energy-axis reparametrization. For each incident-energy index i, we map the energy grid $\{\xi_k = \ln E_{n,k}\}$ to a self-similar coordinate $\kappa_{ik} = \ln(E_{n,k}/E_{p,i}) = \xi_k - \ln E_{p,i}$. This stretch/compression along the outgoing-energy axis removes the artificial under-coverage that occurs if one interpolates directly on E_n or $\ln E_n$ when E_p varies widely.

b. Stage 1: 1D linear interpolation along κ. For each fixed pair (i,j), the discrete points $\{(\kappa_{ik}, \sigma_{ijk})\}_k$ define a piecewise-linear function $\sigma_{ij}(\kappa)$. Given a query (E_p^*, θ^*, E_n^*), compute $\kappa^* = \ln(E_n^*/E_p^*)$. Let k_0, k_1 be such that $\kappa_{ik_0} \le \kappa^* \le \kappa_{ik_1}$. Define

$$\sigma_{ij}(\kappa^*) = (1-\alpha_i)\sigma_{ijk_0} + \alpha_i\sigma_{ijk_1}, \quad \alpha_i = \frac{\kappa^* - \kappa_{ik_0}}{\kappa_{ik_1} - \kappa_{ik_0}}.$$

c. Stage 2: 1D linear interpolation over incident energy. Locate i_0, i_1 with $E_{p,i_0} \le E_p^* \le E_{p,i_1}$ and set

$$\widehat{\sigma}(E_p^*, \theta^*, E_n^*) = (1-\gamma)\sigma_{i_0}(\theta^*, \kappa^*) + \gamma\sigma_{i_1}(\theta^*, \kappa^*), \quad \gamma = \frac{E_p^* - E_{p,i_0}}{E_{p,i_1} - E_{p,i_0}}.$$

d. Stage 3: 1D linear interpolation over angle. For fixed i and κ^*, locate

j_0, j_1 with $\theta_{j_0} \le \theta^* \le \theta_{j_1}$ and set

$$\sigma_i(\theta^*, \kappa^*) = (1-\beta)\sigma_{ij_0}(\kappa^*) + \beta\sigma_{ij_1}(\kappa^*), \quad \beta = \frac{\theta^* - \theta_{j_0}}{\theta_{j_1} - \theta_{j_0}}.$$

This sequential construction is equivalent to a tri-linear interpolant in (E_p, θ, κ), with $\kappa = \ln(E_n/E_p)$. Note that the cross section σ itself is never log-transformed.

By reparametrizing the energy axis with the self-similar coordinate $\kappa = \ln(E_n/E_p)$ (i.e., $k' = \ln(E_n/E_p)$), spectra at different E_p are aligned on a common support so that the query is simultaneously bracketed by both neighboring E_p datasets at the same κ. This alignment enables a straightforward tri-linear interpolation in (E_p, θ, κ) without extrapolation. The interpolation is purely linear; no additional weighting is used beyond the geometric linear fractions α_i, β, γ. Uncertainties from the tensor model are not propagated through the interpolation in this work; interpolated values are reported without error estimates.

C. Geant4 Baseline with BERT

We use Geant4 as an independent, physics-based baseline to benchmark the tensor-model predictions. The standalone source code of the Bertini-style intranuclear cascade (BERT) is not publicly available to us; therefore, we run the reference implementation shipped with Geant4 via a BERT-enabled hadronic physics list and denote the outcomes as "BERT (Geant4)" [12].

BERT (Geant4) describes proton–nucleus spallation through an intranuclear cascade followed by pre-equilibrium, evaporation and fission de-excitation (if relevant) [15]. Elementary reaction cross sections and scattering channels are provided by the Geant4 hadronic package, which allows simulations up to the few-GeV regime. No tuning to experimental data is performed in this work; default model parameters are used.

The scattering neutrons measured in the experiment exhibit specific angular and energy distributions, which are primarily characterized and recorded using DDX. The DDX quantifies the probability that neutrons are emitted into a unit solid angle and within a unit energy interval following the interaction of protons with a target nucleus at a given incident energy. It is a normalized physical quantity representing the average neutron production cross-section per incident proton interacting with a single target nucleus. In contrast, GEANT4 simulation calculations yield the energy and angular information of neutrons emitted from the surface of the scattering target. To derive the DDX of these scattering neutrons, additional post-processing calculations must be performed according to the following formula:

$$\frac{d^2\sigma}{dE_n d\Omega} = \frac{1024 \cdot N_n}{N_p \cdot N \cdot x \cdot \Delta E_n \cdot \Delta\Omega}$$

where $d\Omega = \sin(\theta) \cdot d\theta \cdot d\phi$. Among them, the left side of the equation represents the DDX in units of b/Sr/MeV, while the right side is derived from calculations that convert the number of emitted spallation neutrons into the corresponding DDX. N_p denotes the number of incident protons, $N = \rho N_A / M$ (cm^{-3}) is the number density of target nuclei, x (cm) is the thickness of the thin target, and N_n represents the number of neutrons emitted within a solid angle interval $\Delta\Omega$ in a given scattering direction and within an energy interval ΔE_n (MeV) around a specific neutron energy.

Where experimental DDX data exist, we compare tensor-model predictions and BERT (Geant4) to measurements. In energy-angle regions without measurements, BERT (Geant4) serves as an out-of-sample physics reference to assess the plausibility of the tensor-model interpolation and extrapolation within the admissible domain.

[Figure 1: see original paper]. RMSE as a function of (a) the rank r, (b) the number of iterations N and (c) the discretization interval dEn.

Results and Discussion

A. Selection of Tensor-Model Parameters

We examine three hyperparameters of the tensor model: the CP rank r, the number of Gibbs iterations N, and the logarithmic energy-bin width $\Delta\xi$ used to discretize the outgoing-neutron energy after the transformation $\xi = \ln E_n$ (unless otherwise noted). A smaller $\Delta\xi$ yields more energy bins and denser spectra but also increases sparsity of the tensor and computational cost. Model accuracy is assessed by the root-mean-square error on a logarithmic scale,

$$\mathrm{RMSE}_{\log} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} \left[\ln \left(\frac{\sigma_{\mathrm{pred},i} + \epsilon}{\sigma_{\exp,i} + \epsilon} \right) \right]^2}$$

where n is the number of experimental data points, $\epsilon = 10^{-9}$ b sr^{-1} MeV^{-1} avoids taking the log of zero (not active for our datasets), and all observed points are equally weighted. Unless stated otherwise, RMSE is computed on a held-out mask disjoint from the entries used for fitting.

Figure 1(a) shows $\mathrm{RMSE}_{\ln}$ vs. rank with $\Delta\xi = 0.1$ and $N = 100$. $\mathrm{RMSE}_{\ln}$ decreases with r and saturates for $r \geq 30$. Increasing r from 30 to 50 only improves $\mathrm{RMSE}_{\ln}$ marginally ($0.1418 \rightarrow 0.1406$) while roughly doubling runtime; therefore we adopt $r = 30$ as a practical compromise between fidelity and cost.

Figure 1(b) shows $\mathrm{RMSE}_{\ln}$ vs. the total number of Gibbs iterations N (with $r = 30$, $\Delta\xi = 0.1$). RMSE drops rapidly and stabilizes after $N \approx 50$. We use $N = 100$ to ensure stable posterior means; burn-in is included in N.

Figure 1(c) shows that $\mathrm{RMSE}_{\ln}$ increases with $\Delta\xi$. When $\Delta\xi \leq 0.1$, the $\mathrm{RMSE}_{\ln}$ improvement is modest, but for $\Delta\xi > 0.1$ the degradation accelerates. Figure 2 further compares predictions with data at $E_p = 256$ MeV and $\theta = 7.5°$ for

$\Delta\xi = \{0.05, 0.10, 0.20, 0.40\}$ under $r = 30$, $N = 100$. At $\Delta\xi = 0.05$ the curve shows non-physical oscillations in regions without measurements (both low- and high-energy tails), indicating overfitting to sparse bins despite a slightly smaller $\mathrm{RMSE}_{\mathrm{ln}}$. At $\Delta\xi = 0.20$ and 0.40 the spectrum is over-smoothed and the high-energy peak near the beam-energy region is severely attenuated. $\Delta\xi = 0.10$ best reproduces both the global trend and the peak shape while keeping the computation moderate. Balancing accuracy (Fig. 1), spectral-shape fidelity (Fig. 2), and runtime, we adopt $r = 30$, $N = 100$, and $\Delta\xi = 0.1$ as the default configuration for subsequent analyses.

B. Reproduction of Experimental DDX with the Tensor Model

In this study, 1,727 experimental data points of DDX for spallation neutrons from proton-induced reactions on a natural lead target (EXFOR and relevant literature) were used in full to train the tensor model; we did not split the dataset into training/validation subsets. Accordingly, Figures 3–6 quantify the in-sample reproduction capability of the model rather than out-of-sample generalization. The data span eight incident proton energies from $E_p = 10$ to 3,000 MeV and seven scattering angles from 7.5° to 150°.

Figure 3 summarizes the number of experimental points versus (a) scattering angle θ, (b) incident energy E_p, and (c) neutron energy E_n. A pronounced concentration appears at $\theta = 30°, 60°, 120°, 150°$, with $E_p = 256, 597, 800$ MeV also well sampled; along the energy axis, most measurements lie in $E_n = 1$–10 and 10–100 MeV, whereas the high-energy tail $E_n > 100$ MeV accounts for only 16.2% of all points (Fig. 3(c)). These coverage patterns guide expectations for the reproduction quality: regions with more measurements should be better constrained.

With the optimal hyperparameters fixed from the previous section (r, N, and the logarithmic energy step dE_n), Figure 4 shows tensor-model DDX curves for natural lead at multiple E_p (10–597 MeV) and θ (7.5°–150°). Solid lines indicate kinematics where experimental measurements exist; dashed lines denote settings without corresponding data. Overall, the model reproduces measurements well. For example in Fig. 4(c) ($E_p = 256, 597$ MeV), the predicted curves are smooth and closely follow both the magnitude and shape of the data across the full E_n range. However, when the experimental data points are very sparse, the smoothness of the tensor model prediction curve decreases. In Fig. 4(d) at $\theta = 90°$ for $E_p = 103, 113$ MeV, the high-energy tail fluctuates and the mid-energy segment does not fully pass through the data—consistent with the lower local sampling at these energies/angle. Although the local data points for $E_p = 103, 113$ MeV are fewer than at $\theta = 90°$, the prediction is smoother and better centered on the points, as shown in Fig. 4(e) at $\theta = 120°$. This is attributable to the collaborative filtering mechanism: the total amount of measurements at 120° (Fig. 3(a)) is more than twice that at 90°, so information shared across E_p within the same angle stabilizes the reconstruction. This demonstrates that the collaborative filtering algorithm can effectively leverage relevant experimental information to capture intrinsic physical trends, even in the absence of explicit physical equations.

Across Fig. 4(c)-(f), as E_p increases and coverage improves (Fig. 3(b)), both smoothness and shape fidelity are noticeably enhanced. This further confirms the positive correlation between model performance and the size of the available sample.

To assess agreement uniformly across orders of magnitude, we analyze the prediction-to-experiment ratio

$$r = \frac{\sigma_{\mathrm{tensor}} + \epsilon}{\sigma_{\mathrm{exp}} + \epsilon}, \quad \epsilon = 10^{-9}\ \mathrm{mb\ sr}^{-1}\mathrm{MeV}^{-1},$$

where ϵ prevents division by zero in vanishing tails; points with $\sigma_{\mathrm{exp}} < \epsilon$ are masked in ratio plots. Figure 5 reports r versus (a) θ, (b) E_n, and (c) E_p over all 1,727 points. Most ratios cluster around 1 and lie within 0.6–1.4. A ratio greater than 1 indicates overestimation by the model, while a ratio below 1 indicates underestimation. The spread tends to be smaller at angles with richer coverage (e.g., 60°, 120°), and broader where the coverage is poorer when combined with high-energy tails. Larger deviations concentrate at $E_n > 100$ MeV (Fig. 5(b)), consistent with Fig. 3(c) where only 16.2% of points lie in this range. At well-sampled E_p (e.g., 256, 597 MeV) the ratios are tightly distributed, while at sparsely sampled E_p (e.g., 103, 113 MeV) the spread increases—matching the behavior seen in Fig. 4(d).

Figure 6 summarizes the ratio statistics with a histogram bin width of 0.025. Overall, 96.3% of points fall within $0.8 \leq r \leq 1.2$ (within ±20%), 80.6% within $0.9 \leq r \leq 1.1$ (±10%), and 52.46% within $0.95 \leq r \leq 1.05$ (±5%). The distribution centers near $r = 1$ with modest tails; the outlying bins are mainly associated with the sparsely sampled high-energy region $E_n > 100$ MeV noted in Fig. 3(c). These statistics, together with the qualitative overlays in Fig. 4, indicate strong in-sample agreement and support the reliability of the tensor model in reproducing DDX across diverse kinematics.

C. Analysis of the Prediction Effect of the Tensor Model on the Cross-Section

To date, the discussion has primarily focused on the model's ability to reproduce experimental data and its associated performance. However, a comprehensive evaluation of the model's effectiveness requires further assessment of its accuracy in predicting DDX in the absence of corresponding experimental data—a key aspect for evaluating its generalization and predictive capabilities.

Typically, model predictions are validated by comparison with data from nuclear databases. However, in this study, for the DDX predicted by the tensor model in the absence of corresponding experimental measurements, no relevant evaluated data were available in the five major evaluated nuclear data libraries (ENDF/B, JEFF, ROSFOND, JENDL, and CENDL). Therefore, we employ the Bertini intranuclear cascade model as implemented in Geant4 to simulate the spallation reaction, using its results as a physics-based reference for comparative analysis. Where applicable, we also refer to results from the high-precision variant reported in the literature [BERT HP, Ref. [25]] for additional cross-validation.

. Geant4 simulation parameters of spallation reactions induced by proton bombardment of natural lead thin targets

Incident energy / MeV	Radius / cm	Thickness / cm	Density / g · cm ^{3}

Firstly, it is necessary to ensure that the Geant4 program is used reasonably and reliably for simulating proton-induced spallation reactions. To verify the reliability of the Geant4 setup, this work utilized BERT (Geant4) to calculate the DDX of spallation neutrons at multiple scattering angles for proton bombardment of a thin natural-lead target at incident energies of 113 MeV, 256 MeV, and 597 MeV. These results were compared with the corresponding experimental data and with the BERT HP results in the literature [25]. The number of incident protons in each Geant4 run was $N_p = 10^8$ (to control statistical fluctuations); the thin-target parameters are given in Table 1. The conversion from neutron counts to DDX follows Eq. (10) using the same ΔE_n and $\Delta\Omega$ bin widths as the experimental/tensor-model grids.

Figure 7 compares the calculation results of BERT (Geant4) in this work with the corresponding experimental values, the BERT HP results in Ref. [25], and the tensor-model predictions at the same (E_p, θ, E_n) points. As analyzed in the previous section, the tensor-model curves closely match the experimental data. The overall trend of BERT (Geant4) is consistent with the measurements, but its reproduction shows larger deviations than the tensor model where data are dense. Specifically, for multiple angles at $E_n < 20$ MeV the BERT (Geant4) calculations agree well with experiments and reproduce the small-angle peak (e.g., $\theta = 7.5°$). In the range $E_n = 20$–100 MeV, BERT (Geant4) tends to underestimate the cross section. For example, at $E_p = 113$ MeV and $\theta = 30°$, the deficit relative to data can reach 70%. As the incident energy increases, the deviation generally decreases.

Furthermore, as shown in Fig. 7(b), the BERT (Geant4) results in this work and the BERT HP results in Ref. [25] are in good overall agreement. Below 20 MeV, their reproduction of the experimental data is similar. At very large angles (e.g., 150°), both models underestimate the 20-100 MeV region, with BERT HP slightly closer to data. Taken together, these checks support the use of BERT (Geant4) as a reasonable physics baseline for out-of-measurement comparisons, while recognizing that it is not a substitute for experimental truth.

When the incident proton energies are 113, 256, and 597 MeV, experimental data are missing at some angles (e.g., 7.5°, 15°, 90°, 120°). The tensor model predicts and completes the missing DDX on the same discrete grids. Figure 8 compares the tensor-model predictions (no corresponding experimental points) with BERT (Geant4). Across incident energies and angles, the overall trends are consistent. In the low-energy region $E_n = 1$–10 MeV the two are often very close; in $E_n = 10$–100 MeV moderate deviations appear. For instance, at $E_p = 113$ MeV the tensor model is lower than Geant4 in 10-50 MeV and slightly higher in 50-100 MeV, with the spectral falloff occurring earlier. As E_p increases, these discrepancies decrease. This behavior is consistent with the three-way comparison in Fig. 7 where experimental data exist. Overall, these results suggest that the tensor-model predictions in data-sparse regions are physically plausible relative to an independent baseline.

D. Interpolation Results and Analysis

This section uses the tensor-model DDX for spallation neutrons on natural Pb at the first five incident energies (10-597 MeV) and seven scattering angles (7.5°-150°) as inputs. Interpolation is then applied over proton incident energy E_p and scattering angle θ on fixed energy slices defined by the self-similar coordinate $\kappa = \ln(E_n/E_p)$. Unless otherwise noted, the κ-grid spacing is $\Delta\kappa = 0.2$. The resulting high-resolution database is evaluated on a regular grid with E_p step of 1 MeV and θ step of 0.5°; along the energy dimension, values are obtained at prescribed κ (and, when reporting on a uniform E_n grid, by mapping $\kappa \to E_n$ at the target E_p and linear interpolation in κ). No extrapolation is performed outside the convex hull of (E_p, θ).

Figure 9 illustrates the interpolation across E_p and θ at fixed κ. Only nine representative cases are displayed for illustration. Solid segments indicate kinematics with experimental constraints; dashed segments denote interpolated values where no measurements exist. Overall, the curves are smooth across (E_p, θ) without non-physical oscillations or negative cross sections, and they agree with available measurements at the same kinematics.

The interpolants also follow expected physics trends. In the low-energy region ($E_n < 10$ MeV), all curves show evaporation-like spectra with rapidly decreasing DDX. At higher E_n, forward-peaked features emerge at small angles (e.g., Fig. 9(a)), consistent with anisotropic emission of high-energy neutrons in spallation. As θ increases, the high-energy tail flattens and the peak weakens progressively.

Because the energy axis is parameterized by $\kappa = \ln(E_n/E_p)$ with a finite $\Delta\kappa$, the minimum E_n covered after mapping back from κ depends on E_p. Consequently, some curves may not reach exactly 1 MeV (typical gap 0.6-1.0 MeV). Given that most experiments report from $E_n \geq 1$ MeV, the impact is limited. If needed for downstream use, the gap can be removed by (i) extending the κ-grid toward lower values during preprocessing, or (ii) linearly (or exponentially) extending the spectrum from the first bin above 1 MeV down to 1 MeV, with the filled segment flagged.

The DDX database produced by the tensor model plus bilinear interpolation provides a fine resolution (1 MeV in E_p, 0.5° in θ; and either $\Delta\kappa = 0.2$ or a user-specified E_n grid obtained via κ-linear evaluation). As the five major evaluated libraries lack comparable DDX at the same kinematics/resolution, we also use the Geant4 BERT model as an independent physics reference.

Figure 10 shows the interpolation results at six scattering angles from 10° to 140° for proton incident energies of 113 MeV, 256 MeV, and 597 MeV comparing with the calculations from the BERT (Geant4) model. It is shown that the interpolated curves and BERT (Geant4) results share consistent global trends: high DDX at low E_n with rapid falloff, and a diminishing cascade tail and peak with increasing θ. However, at specific angles and within certain energy ranges, the results obtained from the interpolation method exhibit notable discrepancies compared to those calculated by the BERT (Geant4) model. At $E_n < 10$ MeV, agreement is generally excellent across angles. At $E_n > 10$ MeV, BERT (Geant4) tends to be lower than the interpolation, with the difference growing toward larger θ and diminishing at higher E_p. This is consistent with Fig. 7 and Ref. [25], where BERT (Geant4) and BERT HP systematically underestimate data in the 20–100 MeV region. In the absence of experimental DDX at these kinematics, the interpolated cross sections are therefore reasonable from a physics-consistency standpoint.

Summary

The ADS system is one of the key facilities for managing high-level radioactive nuclear waste. The neutron physics design of its core depends critically on accurate neutron source term data. However, experimental data on the DDX of spallation neutrons remain severely limited, leading to the widespread use of isotropic and fission spectrum approximations in simulations—approximations that may introduce significant errors.

To address this issue, this work employs a Bayesian Gaussian CP (BGCP) tensor model, leveraging data from the EXFOR database and experimental measurements in the literature [15–18], to systematically predict and complete the DDX of spallation neutrons for a natural lead target over $E_p = 10$ MeV–3 GeV and $\theta = 7.5°$–150°. Under optimal hyperparameters for the tensor model—CP rank $r = 30$, total iterations $N = 100$, and logarithmic outgoing-energy discretization $\Delta\xi = 0.1$ with $\xi = \ln E_n$—the model demonstrates excellent in-sample reproduction: 96.3% of points are within ±20% of experiment, 80.6% within ±10%, and 52.46% within ±5%. Where experimental DDX are unavailable, the predictions are checked against an independent physics baseline, BERT as implemented in Geant4. The trends are consistent, especially at $E_n < 10$ MeV; in the 20–100 MeV range, where BERT (Geant4) are known to underestimate data, our predictions remain physically plausible.

Building on the tensor model, we construct a high-resolution DDX database via interpolation over (E_p, θ) on fixed self-similar energy slices $\kappa = \ln(E_n/E_p)$ (default $\Delta\kappa = 0.2$). The database is provided on a regular grid with E_p step of

1 MeV and θ step of 0.5°; along the energy dimension the values are evaluated at prescribed κ and, when needed, mapped back to an E_n grid at the target E_p. No extrapolation is performed outside the convex hull in (E_p, θ), which avoids non-physical oscillations and negative cross sections. Because the minimum E_n after $\kappa \to E_n$ mapping depends on E_p, a small incomplete segment (0.6–1.0 MeV) may appear below 1 MeV; this has limited practical impact since most experiments report from $E_n \geq 1$ MeV. If needed, users may (i) extend the κ-grid toward lower values during preprocessing, or (ii) linearly (or exponentially) extend the spectrum from the first bin above 1 MeV down to 1 MeV.

In summary, this study successfully applies the tensor-model approach to predict spallation-neutron DDX and delivers a validated, high-resolution database for natural lead covering proton energies from 10 to 597 MeV (including the CiADS design point at $E_p = 500$ MeV) and scattering angles from 7.5° to 150°. The method is extensible to other targets and reaction types. For deployment in transport simulations, the database can be directly coupled to Monte Carlo codes (e.g., OpenMC) to provide anisotropic, energy–angle-resolved source terms for subcritical assemblies.

Future work will: (i) incorporate reported experimental uncertainties as entry-wise precisions to account for heteroscedastic noise; (ii) propagate the tensor-model posterior through the interpolation to provide credible intervals on the interpolated DDX; (iii) extend target materials and incident-energy coverage; and (iv) integrate the database into CiADS analyses to quantify impacts on reactivity, power distribution, and transmutation efficiency.

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