3.2.1 ACE Data Manipulations

The A Compact ENDF file (ACE) format is used for nuclear data within MCNP and other monte-carlo codes. It contains all relevant data from ENDF files, support random access of data, and specifies all cross-sections on the same unionized energy grid. The ACE data is a formatted data file and readers are available, though writers tend to only translate ENDF data to ACE, with no general method to manipulate the ACE data directly. The ACE data reader within OpenMC [48] was used to read in ACE files. A writer was created based on the structure of ACE files. All data is represented in contiguous arrays, so that if the original data is known (from reading the ACE data), that data can be searched for within the ACE file and replaced with new values as long as the exact same energy grid is specified. This method of adjusting ACE data is implemented in ASAPy. A few nuances when dealing with different data will be discussed.

Cross-Section Perturbation: Nuclear data sampling occurs using multi-group methods while ACE data is stored in a continuous format. Perturbation factors are generated based on taking a ratio of sampled cross-sections and multi-group average cross-sections. These perturbation factors are then applied to the continuous cross-sections by mapping the multi-group structure on the continuous structure.

ENDF Sum Rules: Many ENDF reactions are subsets of other reactions, so when one cross-section is sampled, others might need to be adjusted for consistency. This is performed within ASAPy by keeping track of all MTs adjusted and comparing against sum rules. Table 3.1 shows the relevant sum rules from the ENDF manual [26].

$\bar{\nu}$ Data: ENDF data allows for inclusion of total, average number delayed, and prompt fission neutrons. MCNP only uses the total values within ACE files, so only these are modified.

Fission χ Spectrum: The distribution of energy of neutrons born from fission depends

on the incident neutron energy. As such, ACE data file stores several tables for a few incident neutron energies. ENDF covariance data does not have covariance data for each incident neutron so the covariance data within the ENDF file is applied to all incident neutron energy distributions. The distributions are also stored as probability and cumulative distribution functions (PDF and CDF). To sample these, the PDF is perturbed then the CDF is adjusted based on the PDF perturbations then the CDF is renormalized by adding up the original PDF and perturbation factors to ensure the CDF sums to 1.

3.2.2 Covariance Data

The most comprehensive resource for covariance data is distributed within SCALE 6.2 [21]. It combines covariance data from several nuclear data sources and experiments. A fine 252-group and coarse 56-group structure is available within SCALE. An older 44-group structure exists but contains old data that is not recommended for use. The covariance data can be converted from the internal SCALE binary format to a ASCII format using the SCALE tool AmpxCOVConverter. The resulting data file contains data for material numbers and their relevant reactions correlated with one another. The standard deviations of the specified reactions are given in the relevant group structure followed by the actual correlation matrix. A covariance parser was created within ASAPy to convert the ASCII file to a more general HDF5 store with a hierarchy based on: '/mat1/mt1/mat2/mt2' corresponding to data correlating mat1 MT1 with mat 2 MT2. Often mat 1 and mat 2 are the same, and MT1 and MT2 are the same, specifying self-correlation. Any group structure can be accommodated by the parser such that new evaluations can be easily used within ASAPy.

Covariance data also exists in ENDF files and these covariances can be used to create any group structure as well as use any weighting flux to create covariance matrices to sample with. The SCALE based data was generated using a typical LWR flux that in-

clude a thermal, epi-thermal, and fast region. ENDF data can be parsed with NJOY [27] to generate covariance data. ASAPy implements NJOY input writers along with ENDF readers to minimize the amount of user input to generate covariance data. The minimum input is a path to an ENDF file and the reaction MT numbers to generate covariance data for. A BOXER format reader was also generated in order to read the BOXER formated covariance files into the previously described HDF5 format.

The covariance data comes in multi-group format which must be mapped to relevant continuous energy bins in ACE data. After sampling data within the multi-group structure, the data is divided by the multi-group mean cross-section to calculate a relative cross-section. These cross-sections are mapped onto the continuous energy group bins then multiplied by the ACE data to generate a sample of data. Two assumptions made are that the group-mean values within the data are very similar to the mean values within the ACE data and that the data within an energy bin are fully-correlated with one another.

3.2.3 Sampling Techniques

A slight deficiency in the ENDF format is the inability for evaluators to convey what type of distribution covariance data should take. Often physical parameters like cross-sections cannot take negative values, but assuming normal distributions are assigned to reported covariances, negative values are possible. An approach often taken is to discard negative data, biasing the sampling scheme. Another method is to assume the distributions are log-normal, which always has positive values. However, without knowing what distributions the covariance data were specified for, errors can occur when large relative errors are present with strong negative correlations [49] due to not transforming the normal-cov to lognormal-cov. In this dissertation, ENDF covariance data is transformed to log-normal covariance data then log-normal sampling is performed ensuring no negative samples are taken.

Nuclear data has strong correlations between energy groups so when sampling data, the full covariance of the data must be taken into account. Multivariate-normal distributions allow for sampling of such data. Given a desired covariance matrix, C, that is semi-positive definite, and mean values, μ, a multi-variate sample, X_i can be generated as follows. First draw uncorrelated values from the mean using a standard-normal distribution, $\mathcal{N}$ and place the means in a diagonal matrix,

$$x_i = \mathcal{N}[\mu = 0, \sigma = 1],$$

then perform a singular value decomposition of the covariance,

$$C = USV, \tag{3.4}$$

where U and V are orthogonal matrices, and S is a diagonal matrix containing the singular values of C. A sample can then be drawn as

$$X_i = \mu + x_i S^{0.5} v$$

This method is implemented in Scipy [50] within np.random.multivariate_normal. One may also use eigen or Cholesky decomposition instead of singular value decomposition with similar results.

ENDF based nuclear data sometimes is published with non-semi-positive-definite covariances. In this case the correlation data R must be manipulated to draw samples. An eigen-decomposition of the correlation matrix is made,

$$R = Q \Lambda Q^{-1},$$

where Q contains the eigenvectors of R, and Λ contains the eigenvalues on the diagonal. The negative eigenvalues are set to a small positive number (1e-8) to form $\tilde{\Lambda}$ then the original eigenvectors are multiplied back in to form an adjusted correlation matrix, $\tilde{R}$,

$$\tilde{R} = Q\tilde{\Lambda}Q^{-1}.$$

The correlation matrix is used due to smaller spreads in eigenvalues, however often the small eigenvalues imposed on the matrix cause numerical difficulties when converting the correlation matrix to a covariance matrix so the above procedure may need to be repeated on the created covariance matrix.

A second method based on a partial Cholesky decomposition [51] that generates a positive semi-definite matrix that equals the original matrix minus an error term was also implemented for correcting non semi-positive definite matrices.

A non-semi positive definite correlation example is the correlation matrix for (n, γ) cross-section of ^{184}W within ENDFB/VIII. The eigen-decomposition and partial Cholesky algorithms were applied to generate 500 samples and the correlation matrices are shown in Fig. 3.3, where it can be seen that both algorithms perform well compared to the original correlation matrix.

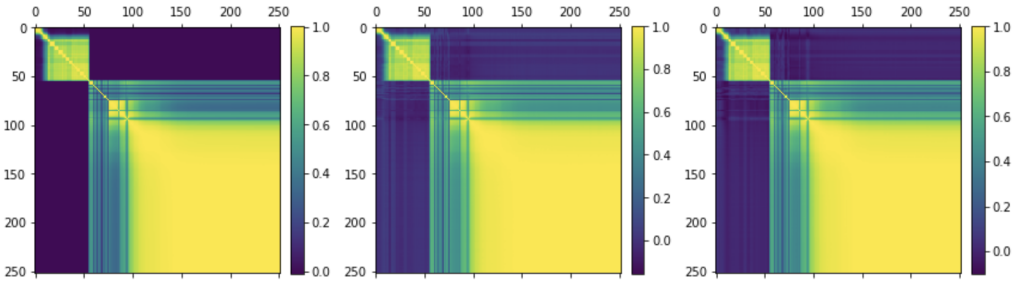

Figure 3.3: Correlation matrices from (left) the evaluated data file (middle) eigen-decomposition sampling (right) partial Cholesky decomposition sampling