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Preliminary Covariance Data Representation for the "A Compact ENDF" File

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INTRODUCTION

In typical applications in criticality, the most important contributor to the uncertainty of the effective multiplication factor k is from the uncertainties in the nuclear data or cross sections. Over the last few decades, there has been increasing efforts by the nuclear data evaluators to provide covariance data for libraries such as ENDF [1]. Data processing codes such as NJOY [2] have been able to process various ENDF covariance formats for almost as long. Sensitivity coefficient capabilities, which are necessary for uncertainty propagation, have also been developed in various Monte Carlo code packages [3, 4] such as SCALE [5] or MCNP [6] .

While MCNP6 can currently compute sensitivity profiles, it has no capability for handling the covariance data. Correspondingly, no format currently exists in the "A Compact ENDF" (ACE) format that MCNP requires. Therefore, a new compact format using principal eigenvectors is proposed. The format is discussed. Memory requirements needed to achieve sufficient precision on the uncertainty of k are shown for Pu-239 on a bare, fast metal and a thermal solution system, and U-235/238 on a reflected fast, metal and a thermal lattice system. Early work is shown to develop a methodology to decide a priori how many principal eigenvectors are needed for a covariance matrix reconstruction of sufficient fidelity.

ACE COVARIANCE FORMAT

Because of the dimensionality of the data and its rapidly growing resolution and fidelity, memory requirements are a concern. Covariance data files for an individual isotope generated by NJOY are typically tens of MB today, but can be expected to grow into the hundreds of MB in the future. When multiplied by the number of isotopes in ENDF, the amount of memory required may reach into the tens of GB. While this clearly will fit on modern machines, it does pose an issue with distribution and installation, especially when considering that data files that are released tend to be so in perpetuity to support user's validation baselines. Also, representing many covariance matrices in RAM during runtime is problematic, so limiting memory footprint is important for that reason as well.

A typical approach for reducing storage requirements is, rather than using the covariance matrices (or upper-triangular representations thereof) directly, to find its principal eigenvalues and eigenvectors, and store only those. While some information is lost, an approximate covariance matrix can be constructed as needed with relatively little computational cost. If enough eigenvectors are kept, the loss of information from reconstructing the matrix should be small and within the uncertainties, approximations, and assumptions of the covariance data itself.

First, the ERRORR module within NJOY is used to process the ENDF file and create an intermediate file. This file has some compression as it decomposes the covariance matrix into reaction (MT) blocks and only stores the relevant, non-zero components of each row.

This file is then processed and the full covariance matrix $\mathbf{C}$ is given to a linear algebra solver (for now MATLAB) to generate its eigenvalues and eigenvectors. The eigenvectors are given as the columns of matrix $\mathbf{V}$ and the eigenvalues along the diagonal matrix $\mathbf{D}$. The file size for all the eigenvalues and eigenvectors is usually many times larger than the original file. Typically, most of the variation can be captured with a smaller subset of eigenvectors, and the required file size is usually smaller than the original NJOY file.

The magnitude of an eigenvalue denotes how much variation occurs along a direction given by its corresponding eigenvector, so some acceptance criteria for how many to use can be made based on them. A possible metric for picking the number of eigenvectors is investigated, but much research remains to be done to determine an appropriate acceptance criteria. Suppose the subset of selected eigenvectors are in matrix $\widetilde{\mathbf{V}}$ and their corresponding eigenvalues are in diagonal matrix $\widetilde{\mathbf{D}}$. The approximate covariance matrix $\widetilde{\mathbf{C}}$ can be reconstructed by

$$\widetilde{\mathbf{C}} = \widetilde{\mathbf{V}}\widetilde{\mathbf{D}}\widetilde{\mathbf{V}}^T \tag{1}$$

The subset of eigenvalues and eigenvectors are stored in the ACE covariance format.

The ACE covariance format is an array consisting of four sections of information. The first section contains the number of energies followed by the energy grid in ascending order. The second is a list of ZAID's and reaction MT's for the blocks of the matrix. Third is the number of eigenvalues kept and a list of those eigenvalues in order of decreasing magnitude. The fourth contains the eigenvectors in a compact form.

Because of the nature of the covariance matrix, the eigenvectors often have long, contiguous zero-valued segmets. Rather than storing the entire eigenvector, a simi-

lar format to what is used in the NJOY file is employed. For each eigenvector, the number of non-zero segments is stored; and for each segment, the starting location, number of elements in the segment, and the elements themselves are given. Doing this further compresses the ACE covariance data.

COMPRESSION RESULTS

The ENDF covariance file for Pu-239, U-235, and U-238 are processed by NJOY to produce its own file. This file is processed into a format MATLAB can read, and that program is used to generate all the eigenvalues and eigenvectors. These are output into files that are read by an external script that creates an ASCII file for the proposed ACE format. The other input to the script is the number of eigenvectors to store in the proposed format.

To determine the performance of reconstructing the covariance matrix, i.e., how good of an approximation is $\widetilde{\mathbf{C}}$ of $\mathbf{C}$ for a given number of eigenvectors, and how well the uncertainty of k, Δ_k, is estimated. To do this, MCNP6 calculates energy-resolved sensitivity profiles on the energy grids and reactions specified in the NJOY (or ACE) file. The sensitivity of k with respect to nuclear data x over some energy group g is defined as

$$S_{k,x_g} = \frac{x_g}{k}\frac{dk}{dx_g}. \tag{2}$$

If these sensitivities are ordered as the covariance matrix and stored in row-vector $\mathbf{S}$, then uncertainty in k may be estimated by

$$\Delta_k = \mathbf{SCS}^T. \tag{3}$$

This is the best possible estimate of Δ_k for a given sensitivity vector and covariance matrix. Approximate values of the uncertainty in k, $\widetilde{\Delta_k}$ may be obtained using $\widetilde{\mathbf{C}}$ as opposed to $\mathbf{C}$. There error $\mathcal{E}$ for estimating the uncertainty is given as

$$\mathcal{E} = 1 - \frac{\widetilde{\Delta_k}}{\Delta_k}. \tag{4}$$

Pu-239

The Pu-239 covariance data produced by NJOY (processed form ENDF/B-VII.1) has a unionized energy grid of 476 groups, treating the reactions of total, elastic, inelastic, (n,2n), (n,3n), fission, (n,4n), and (n,γ). The size of this file is 18 MB. For the compression scheme to be effective, the ACE formatted data should be of significantly less size than the NJOY data (which is taken to be "exact") with as small a possible $\mathcal{E}$.

Sensitivity profiles are generated for two ICSBEP [7] benchmarks: pu-met-fast-001 (Jezebel or PMF1) and pu-sol-therm-009 (PST9). These represent two ends of the fission producing energy spectrum, with the former being a bare, fast metal system and the latter being a thermal solution system. These sensitivity vectors are loaded into MATLAB and used with the full covariance matrix $\mathbf{C}$ to determine the reference Δ_k. Also in MATLAB, various $\widetilde{\Delta_k}$ are calculated based on approximate covariance matrices $\widetilde{\mathbf{C}}$ for numbers of eigenvectors N, along with the error $\mathcal{E}$. The estimated Δ_k for PMF1 is 0.005568, and for PST9, it is 0.007465. Note that the predicted uncertainty does not include fission ν and χ, as this is a "proof of concept" demonstration. Figure 1 shows the error $\mathcal{E}$ in estimating Δ_k for PMF1 and PST9 as a function of the number of eigenvectors employed N. Both show that to get estimates of the uncertainty to within 0.11% of its full covariance value, 200-300 or so eigenvectors are required. The trend with the fast system is that there are long periods where there is little gain in accuracy followed by sharp drops, whereas the thermal system is smoother.

Table I. ACE Covariance Memory Requirements (MB)

$\mathcal{E}$	Pu-239	U-235	U-238
10^{-2}	3.6	6.1	2.9
10^{-3}	4.8	15	5.5
10^{-4}	5.9	19	8.7
10^{-5}	6.0	20	11
NJOY	18	39	43

Table I shows the Pu-239 file sizes of the ACE formatted files to ensure both PMF1 and PST9 can be estimated to within different $\mathcal{E}$. These results show that it is possible to get an approximate covariance matrix that can produce a

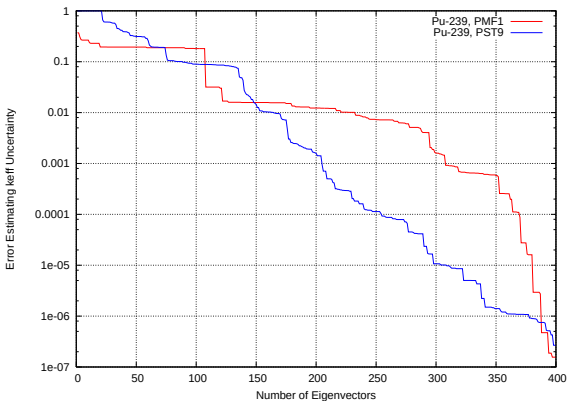

Fig. 1. Number of eigenvalues needed to achieve an error in estimating the uncertainty in k from Pu-239.

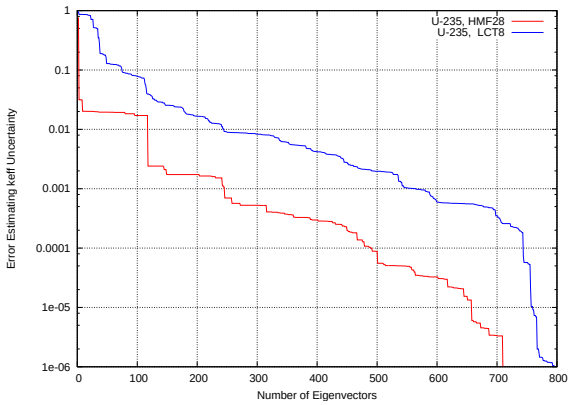

Fig. 2. Number of eigenvalues needed to achieve an error in estimating the uncertainty in k from U-235.

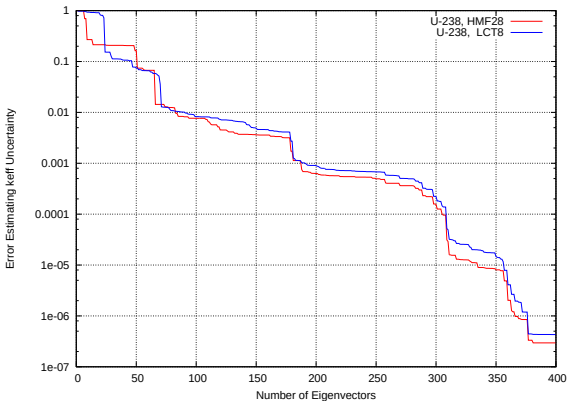

Fig. 3. Number of eigenvalues needed to achieve an error in estimating the uncertainty in k from U-238.

fairly accurate estimate of the Δ_k using a few MB of memory. For instance, to obtain an estimate Δ_k within 0.1%, only 4.8 MB of data are required, which is a savings of over 70% from the NJOY file. Caution should be exercised in taking these conclusions too generally, as they are only based upon k and for only two benchmarks and a subset of reactions; however, this suggests that significant memory savings may be gained by using the proposed principal eigenvector ACE format.

U-235/238

For U-235 with a unionized energy grid of 671 groups, treating the reactions of total, elastic, inelastic, (n,2n), (n,3n), fission, and (n,γ). The U-238 data set has an energy grid of 690 groups, with the same reactions as U-235. Both data are from ENDF/B-VII.1. The file sizes for the NJOY produced U-235 and U-238 files are approximately 39 and 43 MB respectively.

Sensitivity profiles are generated for two ICSBEP benchmarks: heu-met-fast-028 (Flattop or HMF28) and leu-comp-therm-008 (LCT8). These are a U-238 reflected, fast metal system and a thermal lattice physics experiment. These two benchmarks were selected to provide two very different types of spectra, but still be important to the same isotopes.

The same process used for Pu-239 was used for generating U-235/238 results. The estimated Δ_k from U-235 for HMF28 and LCT8 are 0.012022 and 0.002320 respectively. Likewise, the Δ_k from U-238 are 0.003938 and 0.002607.

Figures 2 and 3 give the equivalent results as Fig. 1, but for U-235 and U-238 respectively. This time, the trend is different, with the thermal system requiring many more eigenvectors to accurately resolve Δ_k. Because it is difficult to assign a physical nature to the eigenvectors, the reasons for this cannot be easily explained.

Table I gives the corresponding memory requirements for compressed U-235 and U-238 ACE formats. The U-235 covariance data appears more difficult to compress for these two benchmarks. Getting to the same 0.1% error in Δ_k allows for a compression of 60%, which is still significant. U-238, on the other hand, appears to compress much better; getting an 0.1% error can be done with a memory savings of over 85%. At this time, it is not known whether the amount of compression allowed is because of the nature of the benchmarks, because of the covariance data, or some combination thereof.

RESIDUAL VARIABILITY

The question of how many eigenvectors to keep (or, conversely, what N to truncate) is still open. For a specific set of applications, it is possible to determine reasonable bounds for how large N needs to be. This presents a challenge for a general-purpose data set, which MCNP, being a general-purpose Monte Carlo code, to address. The question that remains to be answered is whether or not some appropriate N can be found for a broad class of neutronics problems. This cannot be answered yet, but it is possible to try and devise a metric for determining N.

Recall that the eigenvalue corresponds to the amount of variability along its eigenvector given direction. By capturing a large amount of the variability, it should be possible to create a $\widetilde{\mathbf{C}}$ that handles most applications. Let g be the total amount of variability, which is given by the sum of all positive eigenvalues (neglect small negative eigenvalues that appear because of numerical issues) of $\mathbf{C}$. Also, g_N is the amount of variability captured by N eigenvalues, or the sum of the first N eigenvalues (all must be positive). Define the residual fraction of variability $\mathcal{R}$ as

$$\mathcal{R} = 1 - \frac{g_N}{g}. \tag{5}$$

Table II. Maximum $\mathcal{E}$ for Given $\mathcal{R}$

$\mathcal{R}$	Pu-239	U-235	U-238
10^{-3}	1.3×10^{-2}	8.9×10^{-3}	1.1×10^{-2}
10^{-4}	8.6×10^{-4}	1.1×10^{-3}	9.0×10^{-4}
10^{-5}	7.5×10^{-7}	3.2×10^{-4}	3.4×10^{-7}

As N approaches the total number of positive eigenvalues, $\mathcal{R}$ approaches zero. The value of N is therefore chosen such that $\mathcal{R}$ is less than some small value. Given the previous results, it is possible to observe a trend between $\mathcal{R}$ and where $\mathcal{E}$ becomes negligible.

Table II contains the values of the highest $\mathcal{E}$ as a function of $\mathcal{R}$ for the isotopes. From these it appears that a threshold of $\mathcal{R} < 10^{-4}$ makes it so Δ_k can be estimated to about 0.1% or less. The hope is that these results are conservative enough for most applications. That said, before actually generating production ACE covariance data, numerous other benchmarks, and using results other than k, will be necessary to ensure the choice(s) of $\mathcal{R}$ is suitably robust. Nonetheless, this does provide hope that there is a methodology for automatically choosing N.

Given $\mathcal{R} < 10^{-4}$ and the number of eigenvectors, the memory savings from the NJOY file can be calculated. For Pu-239, U-235, and U-238 these are 72%, 65%, and 86% respectively. If it turns out for a broad set of applications that the choice of $\mathcal{R}$ is appropriate, then it illustrates that a significant reduction in memory requirements is still possible. Whether or not this is true remains an open question.

FUTURE WORK

The work in generating ACE covariance libraries is just beginning, but the results are suggestive a path forward using principal eigenvectors. Before this is employed, much work remains to be done. More realistic covariance files need to be generated incorporating more data (e.g., fission ν), and many more isotopes are needed. Hopefully, the major actinides presented here represent the more difficult cases, but this remains to be seen. Also, a much larger set of benchmarks need to be assessed to ensure that the number of principal eigenvectors kept is appropriate. The ACE covariance libraries need to be robust enough to handle a very broad range of applications, as MCNP is a general purpose code.

If it turns out these preliminary conclusions are generally true, then the ability to generate the ACE formatted covariance data will need to be integrated directly into NJOY. Once the ACE data is available in the files, then MCNP6 will need to be modified to automatically generate appropriate sensitivity profiles and perform uncertainty quantification. For the near term, this will likely be restricted to k, but the hope is to eventually extend these methods to more general responses.

Another question that needs to be addressed in the near term is what needs to be done in terms of handling secondary distributions. Covariance data exists for fission χ and some angular scattering distributions, which are functions of incident neutron energy. What representation is appropriate and how to handle correlations between incident energies for those data remains to be decided.

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