

Proposed ACE Covariance Format, Version 1.0

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A new ACE format for covariance data is proposed. Rather than storing an upper triangular matrix, the principal eigenvalues and eigenvectors of the matrix for an isotope are stored. The eigenvectors are used by MCNP6 to reconstruct an approximate covariance matrix. The matrix consists of blocks corresponding to ZA/MT pairs. Each block uses the same unionized energy grid. The information is stored into a contiguous block of information in an array called XSS. The array JXS(.,ISOTOPE) gives the pointer to the start of the covariance block for that isotope.

Covariance Block in XSS

PTR	Pointer to the location of another covariance matrix for this isotope.
FMT	Index for the format type. This current type is FMT = 0. The reason for this is to allow for future formats to cover extensions and future needs. JXS points here.
NB	Number of ZA/MT blocks in the matrix. Each block is a matrix with the same energy grid defined later.
MF_1 ... MF_NB	List of ENDF MF numbers for each block (MF = 31 is COV/NU, 33 COV/SIG, etc.).
[ZA_MT]_1 ... [ZA_MT]_NB	Information about ZA/ MT, etc., format depending on the MF type, see below.
NE	Number of energy grid points.
E_1 ... E_(NE+1)	Energy grid bounds. (absent if NE = 0)
NV	Number of eigenvalues stored.
EVL_1 ... EVL_NV	List of eigenvalues. Any order, but eigenvectors must correspond.
[EVC]_1 ... [EVC]_NV	Compressed eigenvectors. See below.

The form for the ZA_MT section is depends on the MF. The three cases are as follows:

ZA_i MT_i	MF = 31/33 is a ZA, MT pair.
ZA_i MT_i NLEG NIE_i IE_(i,1) ...IE_(l,NIE_i+1)	MF = 34 has a ZA, MT pair and is followed by the number of Legendre coefficients and an incident energy grid. For MF = 34, the number of elements in the matrix for this block is NLEG*NIE_i.
ZA_i MT_i NIE_i IE_(i,1) ... IE_(l,NIE_i+1)	MF = 35 has a ZA, MT pair and is followed by an incident energy grid. The number of elements in the matrix for this block is NE*NIE_i.

Note that all outgoing energies and scattering cosines from Legendre moments for direction cosines are to be taken in the center-of-mass frame, like the data in most of the other MCNP formats. For MF 34 and 35, the ordering of the data are major in incident energies, e.g., for MF = 35 a matrix representing all outgoing energies is present for each incident energy. There is no format for MF = 36 (correlated energy-angle) here because the ENDF6 format does not have one either.

The eigenvector is stored in a list of data given in EVC_i. This is done so as not to store zero values. This is done by storing non-zero “segments” of information. Each eigenvector i has the following:

NSEG_i	Number of non-zero segments in EVC_i. The index for the segment is j.
START_(i,j) NUM_(i,j) V_(i,j,1) ... V_(i,j,NUM_(i,j))	Each segment j of eigenvector i consists of the starting non-zero position, and the number of non-zero elements. A list of eigenvector elements in the segment is then given. This is repeated for each segment of this eigenvector.

The eigenvalues and eigenvectors are those of the relative covariance matrices and are averaged over the width of the energy bin.