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Title: Covariance Data File Formats for Whisper-1.0 & Whisper-1.1

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1.0 Introduction

Whisper is a statistical analysis package developed in 2014 to support nuclear criticality safety (NCS) validation [1-3]. It uses the sensitivity profile data for an application as computed by MCNP6 [4-6] along with covariance files for the nuclear data to determine a baseline upper-subcritical-limit (USL) for the application. Whisper version 1.0 was first developed and used at LANL in 2014. During 2015-2016, Whisper was updated to version 1.1 and is to be included with the upcoming release of MCNP6.2.

This report describes the file formats used for the covariance data in both Whisper-1.0 and Whisper-1.1.

1.1 Background

The covariance data for the nuclear cross-sections that are included with Whisper-1.0 and Whisper-1.1 are based on the "Low-Fidelity Covariance Project," a joint effort involving the Brookhaven, Los Alamos, and Oak Ridge National Laboratories that was completed in 2008 [7]. The goal of the project was to provide a complete set of covariance data estimates for all ENDF/B-VII.0 isotopes for elastic scattering, inelastic scattering, (n,2n) reactions, radiative capture, and nubar & fission cross-sections over the energy range 10^{-5} eV to 20 MeV. The covariance data were produced for all 393 isotopes in ENDF/B-VII.0 in a 44-group energy structure. The data are often referred to as "low-fi" or "BLO" data. The goal was to provide completeness, not high fidelity [7]. The data were first used in the SCALE/TSUNAMI system from ORNL [8,9] and included with SCALE-6.0. The recent version of SCALE-6.2 includes the low-fi covariance data as well as new high-fidelity covariance data. Efforts are also ongoing at LANL and other laboratories to produce more high-fidelity covariance data. Such high-fidelity covariance data will be incorporated into future versions of Whisper. For now, only the low-fi data are used.

2.0 Covariance Data File Format for Whisper-1.0

Whisper-1.0 was used only at LANL and Sandia National Laboratory. The description of the file format for covariance data given in Table 1 is only useful for historical purposes, to document the data used during 2014-2016. For definiteness, the data format will be referred to as the "BCK" format.

Table 1. BCK Format for Covariance Data, for Whisper-1.0

- One file for each ZA
  - ZA = Z*1000 + A, or a string (for S(alpha,beta) covariance data)
  - Filenames: cov.ZA.dat
  - ZA must be 6 characters or fewer, with no ID suffix
  - Examples: cov.92235.dat, cov.lwtr.dat
  - ZA1 & ZA2 below follow the same 6-char rules.
- Relevant MTs, list of 12:
  - 2, 4, 16, 18, 102, 103, 104, 105, 106, 107, 452, 1018
- NG = number of groups
  - The NG+1 energy bounds for the groups are stored from high-energy to low-energy in the file. Whisper ignores these, using its own energy bounds (that match) ordered from low-energy to high-energy.
- NCOV = number of NG*NG covariance matrices
  - Despite having information for Coverx-style data compression, Whisper can only use data stored as a full matrix.
  - The covariance matrices are stored in the file with both rows and columns ordered from high-energy to low-energy. After reading the matrix, Whisper reverses the ordering for all rows and columns (i.e., flip left-to-right and top-to-bottom)

```
k1 = 1
do j=NG,1,-1
  k2 = k1 + NG -1
  M( NG:1:-1, j ) = CovData( k1:k2 )
  k1 = k2 + 1
enddo
```

- File format for a given ZA:

```
ZA (6 char), NG, NCOV
( erg(i), i=1,NG+1 )                          NOT USED
( ZA1(i),MT1(i),  ZA2(i),MT2(i), i=1,NCOV )
for i = 1, NCOV
      ZA1(i), MT1(i),  ZA2(i), MT2(i)
      (Map(j,i), NRow(j,i), j=1,NG)           NOT USED
      (CovData(j,i),        j=1,NG*NG)
```

3.0 Covariance Data File Format for Whisper-1.1

Whisper-1.1 makes use of covariance data obtained from ACE covariance files. While the format for NJOY-generated ACE covariance data files is currently under development [10], the description provided here in Tables 2 & 3 is considered "Rev-1," and is what is currently used with Whisper-1.1.

Table 2. Data structure and file format for ACE covariance data, Rev-1

Data structure:

```
type ace_data
  character(len=10)     :: zaid
  real(8)               :: awr
  real(8)               :: temp
  character(len=10)     :: date
  character(len=80)     :: info
  integer(4)            :: iz(16)
  real(8)               :: az(16)
  integer(4)            :: nxs(16)
  integer(4)            :: jxs(32)
  real(8), allocatable  :: xss(:)
end type ace_data

integer(4), parameter :: ACE_COVAR_FORMAT_REV = 1
```

File format for ACE covariance file, Rev-1:

```
    zaid, awr, tmp, date        a10, es12.5, es12.5, a11
    info (comment)              a80
    (iz,az, i=1,16)             4(i7,f11.0)
    nxs(16)                     8i9
    jxs(32)                     8i9
    xss()                       4es20.12
```

- The ZAID is limited to 10 characters – a 6-digit integer or a 6-character string (for S(alpha,beta) identifiers), followed by a suffix of the form ".nnv", where nn is a 2 digit version number, and the letter "v" indicates that the file contains covariance data.
- The entries for `awr, tmp, date, iz(16), az(16)` are not used by Whisper-1.1.
- Details for `nxs(16), jxs(32),` and `xss()` are provided in Table 3.
- Examples of ZAID and corresponding filenames:

  1001.01v, 92235.01v, lwtr.01v, h-zr.01v

Table 3. nxs(), jxs(), & xss() details for ACE covariance data, Rev-1

- Energies & covariance data are ordered in traditional MCNP-style, from low-energy to high-energy.

```
nxs():
     1     nxss,            length of xss()
     2     ZA,              ZA = Z*1000+A  (0 if nonnumeric)
     3     F,               ACE file format revision number =1
     4     ng,              number of energy groups
     5     nxsec,           number of unique za-mt xsec sets
     6     ncov,            number of covariance data sets
     7     covtype          1=absolute, 2=relative, 3=correlation

 jxs():                     location in xss() of:
     1     ix_erg,          energy block
     2     ix_xs_zamt,      za-mt list for xsec's
     3     ix_xs_data,      xsec+std sets for za-mt's
     4     ix_cov,          covariance info list
     5     ix_cov_data      covariance matrix data

 xss():
     ix_erg           erg(1:ng+1)
                      energy bounds for groups, increasing order

     ix_xs_zamt       zamt(3,nxsec)
                      za,mt,wflag for xsec+std data

     ix_xs_data       xsdat(1:ng,2,nxsec)
                      1=xsecs, 2=stds

     ix_cov           covinfo(7,ncov)
                      integers or strings, stored as real*8

          covinfo(1,i) = za1       6-char string, stored in real8
          covinfo(2,i) = mt1
          covinfo(3,i) = za2       6-char string, stored in real8
          covinfo(4,i) = mt2
          covinfo(5,i) = fcv       flag for type of data
          covinfo(6,i) = isparse   flag for full/sparse storage
          covinfo(7,i) = ix_dat    location in xss() of covar data

          fcv:
               31 = nu-bar   covar   (MT=452)
               33 = xsec     covar   (MT=1:451, 453:999)
               35 = chi dist covar   (MT=1018)
          isparse:
               1 = full matrix
               2 = coverx format, bck format
               3 = CCS format
               4 = CRS format

     ix_cov_dat       covar_data(:)
```

3.1 Discussion of ZA restrictions for ACE-covar-Rev1

While there are plans to expand the ZAID naming convention used by MCNP and Whisper, both MCNP6.2 and Whisper-1.1 adhere to the traditional limits:

- The total length of a ZAID is 10 or fewer characters.
- The "/" character may no longer be used in a ZAID, since the ZAID is normally used as the data file name.
- The suffix for ACE covariance data has the form ".nnv".
- The ZA name is 6 or fewer numeric digits for ordinary cross-section data, or a 6-character string for S(alpha,beta) data.

Future versions of MCNP and Whisper will deal with extensions of the ZAID naming convention, most likely to the proposed 24-character form.

3.2 Storing 6-character ZA names in 8-byte real numbers stored in xss()

In Fortran-2003, the intrinsic function ichar() returns an integer corresponding to a particular character. For example, k=ichar(' ') results in k=32 (the numeric code for a blank), and k=ichar("a") results in k=97. All characters used as ZA names and part of filenames are in the numeric range 32-127, requiring 7-bits of storage. Packing 6 characters with 7 bits each into an 8-byte integer produces a 42-bit integer, which requires 13 decimal digits (or fewer). This integer can be stored as an 8-byte real without rounding or truncation. However, since ACE files are distributed in formatted text form, it is essential to use a printing format that retains at least 13 significant digits. In the past, the xss() data were printed using (4es20.11), which is not sufficient. For ACE covariance data (Rev 1), the printing format must be (4es20.12) to avoid rounding or truncation of data containing packed 6-character strings.

Character position in string:	6	5	4	3	2	1
Bits (in 8-byte integer):	35-41	28-34	21-27	14-20	7-13	0-6

Trailing blanks (i.e., possibly character 6, or 5, etc.) are not stored; the corresponding bits are set to zero. Also, ZA names may not contain embedded blanks or characters that are not legal in filenames. Routines in Whisper-1.1 that read or write ACE covariance files (Rev 1) pack or unpack the 6-character ZA strings when the data are read or written.

3.3 Storage formats for Covariance Matrices

Whisper-1.0 and Whisper-1.1 do not make use of compressed storage schemes for sparse matrices. This is appropriate for the current low-fidelity covariance data in 44-group format, but will need to be extended in the future when high-fidelity covariance data is available. Thus, ACE covariance format (Rev 1) need only deal with full matrix storage. In the future, it is likely that the Scale/coverx, compressed column storage (CCS), compressed row storage (CRS), or other sparse storage schemes will be incorporated into both the ACE covariance format and Whisper.

3.4 ZA correspondence between ACE and SCALE naming conventions

Table 4 lists the correspondence between the ZA names used by convention for ACE data and the "material names" used in the SCALE system. For most cases involving ordinary cross-section data, the ACE & SCALE conventions are the same, e.g., 92235 is used in each. Table 4 lists the exceptions, that involve data for metastable states or S(alpha,beta).

Acknowledgments

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References

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Table 4. ACE ZA vs SCALE materials

Scale mat	ACE za	Comment
1801	1001	
8001001	1001	
1802	1002	
8001002	1002	
27601	27458	Co-58m
1027058	27458	Co-58m
47601	47510	Ag-110m
1047110	47610	Ag-110m
48601	48515	Cd-115m
1048115	48515	Cd-115m
52601	52527	Te-127m
1052127	52527	Te-127m
52611	52529	Te-129m
1052129	52529	Te-129m
61601	61548	Pm-148m
1061148	61548	Pm-148m
67601	67566	Ho-166m
1067166	67566	Ho-166m
95242	95642	Am-242 - lanl oddity
95601	95242	Am-242m - lanl oddity
1095242	95242	Am-242m
95611	95644	Am-244m
1095244	95644	Am-244m
1099254	99654	Es-254m

Scale mat	ACE za	Comment
S(alpha,beta) covariances		
1001	lwtr	
1002	hwtr	
1701	h-zr	
1901	poly	
4309	be	
6312	grph	
40701	zr-h	
1001001	lmeth	
2001001	smeth	
4001001	hortho	
5001001	hpara	
6001001	benz	
7001001	h-zr	
9001001	poly	
4001002	dortho	
5001002	dpara	
3004009	be	
5004009	be-o	
3006000	grph	
5006000	benz	
1008016	o2-u	
5008016	o-be	
1013027	al27	
1014028	sio2	
1014029	--	si29o2
1014030	--	si30o2
1026000	fe56	
1040090	zr-h	
1040091	--	zr91-h
1040092	--	zr92-h
1040093	--	zr93-h
1040094	--	zr94-h
1040095	--	zr95-h
1040096	--	zr96-h
1092235	u-o2	

Scale mat numbers obtained from Scale-6.0 manual & 6.2 manual table 7.2.1, 7.2.3, 10.1.1, 10.2.1. MCNP za numbers obtained from LA-UR-13-21822 rev4.