ENDSAM manual

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1 Purpose

Program ENDSAM is written in Fortran language. It receives

- a nonnegative number n,

- a file from a nuclear data library of a certain isotope in ENDF-6 format [1].

Then it

- reads mean values of parameters from File 2 in ENDF-6 format,

- reads covariance data of parameters from File 32 in ENDF-6 format,

- gives information about possible inconsistencies,

- makes n new files in ENDF-6 format which contain values of random samples of resonance parameters in places of original values in File 2.

Moreover,

- if $n = 0$, then only the information about possible inconsistencies is given,

- if there is no File 32 in the processed file, then no output files are created.

2 Input file

ENDSAM reads input data from a file named 'Input' which should be of the form

$$\boxed{\begin{array}{l} n \\ File_1 \\ \vdots \\ File_k \end{array}}\,,$$

where n is the number of required samples written in free format and $File_1, \ldots, File_k$ is the list of the files in ENDF-6 format to bo precessed.

An example of such an input file is

```
5
..\neutrons\n-011_Na_023.endf
..\JEFF32N\n-10-Ne-022.jeff32
```
.

3   Restrictions on covariance data

ENDSAM assumes that resonance parameters are governed by the following distributions.

Resonance energy ER : Normal $N\left(\mu, \sigma^2\right)$ with density function $f\left(x\right) = \frac{1}{\sqrt{2\pi}\sigma}e^{\frac{-(x-\mu)^2}{2\sigma^2}}$.

All other parameters except fission width GF : Lognormal $LN\left(\mu, \sigma^2\right)$ with density function $g(x) = \begin{cases} \frac{f(\log x)}{x} & : \quad x > 0, \\ 0 & : \quad x \leq 0. \end{cases}$

Fission width GF :

- If it has positive mean, then lgonormal $LN\left(\mu, \sigma^2\right)$.
- If it has negative mean, then minus lognormal with density function $g\left(-x\right)$.

ENDSAM reads resonance parameters $x_1, \ldots, x_m$ and it applies well-known random sampling methods on a collection of normally distributed parameters

$$\widetilde{x}_j = \begin{cases} x_j & : \quad x_j \text{ is normal,} \\ \log|x_j| & : \quad x_j \text{ is either lognormal or minus lognormal.} \end{cases}$$

While doing so, the following restrictions of lognormal distribution have to be taken into account. If x_j is lognormal or minus lognormal and $\langle x_j \rangle$, $\sigma\left(x_j\right)$ and $\mathrm{ru}\left(x_j\right)$ respectively stand for its mean, deviation and relative uncertainty, then its data transforms in the following way:

Means:

$$\langle \widetilde{x}_j \rangle = \log|\langle x_j \rangle| - \frac{\log\left(1 + \mathrm{ru}\left(x_j\right)^2\right)}{2}$$

Deviations:

$$\sigma\left(\widetilde{x}_j\right) = \sqrt{\log\left(1 + \mathrm{ru}\left(x_j\right)^2\right)},$$

Correlations:

$$\mathrm{cor}\left(\widetilde{x}_i, \widetilde{x}_j\right) = \begin{cases} \mathrm{cor}\left(x_i, x_j\right)\frac{\mathrm{ru}(x_j)}{\sqrt{\log\left(1+\mathrm{ru}(x_j)^2\right)}} & : \quad x_i \text{ is normal,} \\ \frac{\log(1+\mathrm{cor}(x_i,x_j)\mathrm{ru}(x_i)\mathrm{ru}(x_j))}{\sqrt{\log\left(1+\mathrm{ru}(x_i)^2\right)\log\left(1+\mathrm{ru}(x_j)^2\right)}} & : \quad \text{otherwise.} \end{cases} \tag{3.1}$$

It follows from (3.1) that correlations must satisfy

$$e^{-\sqrt{\log\left(1+\mathrm{ru}(x_i)^2\right)\log\left(1+\mathrm{ru}(x_j)^2\right)}} \leq 1 + \mathrm{cor}\left(x_i, x_j\right)\mathrm{ru}\left(x_i\right)\mathrm{ru}\left(x_j\right)$$
$$\leq e^{\sqrt{\log\left(1+\mathrm{ru}(x_i)^2\right)\log\left(1+\mathrm{ru}(x_j)^2\right)}} \qquad (3.2)$$

if both, x_i and x_j are either lognormal or minus lognormal, while in the case when x_i is normal we get

$$\left|\mathrm{cor}\left(x_i, x_j\right)\right| \leq \frac{\sqrt{\log\left(1 + \mathrm{ru}\left(x_j\right)^2\right)}}{\left|\mathrm{ru}\left(x_j\right)\right|}. \qquad (3.3)$$

If correlations satisfy equations (3.2) and (3.3), then it is a step in the sampling method to compute a Cholesky decomposition of the matrix $\widetilde{C} = [\mathrm{cor}\left(\widetilde{x}_i, \widetilde{x}_j\right)]$. Therefore, it is of fundamental importance that this matrix is positive definite. However, in some nuclear data libraries this is not the case. When this happens, ENDSAM first computes the nearest positive definite correlation matrix of $\widetilde{C}$ in Frobenius norm by applying Higham's method [2].

4   Output: information about inconsistencies

ENDSAM throws a warning if any of the following inconsistencies occurs.

- The smallest lower range limit EL for Files 2 and 32 agree, but the highest upper range limit EH in File 32 is greater that that in File 2. In this case energy ranges are treated such as they coincide.

- Given correlation matrix is of size m, but nonzero correlation is given at position (i, j) for $i > m$ or $j > m$. In this case this correlation is ignored.

- A certain parameter has zero deviation, but a nonzero correlation with another parameter. In this case this correlation is ignored.

- A certain parameter has a negative variance or deviation. In this case its sign is changed.

- A certain resonance from File 32 is not found in File 2. In this case parameters of this resonance are not sampled. Resonances are considered to agree if their first parameters coincide up to a relative error of $10^{-3}\%$ and the other parameters coincide up to a relative error of 10%.

- A certain parameter is distributed lognormaly and has nonpositive mean or is distributed minus lognormaly and has nonnegative mean. In this case this parameter is not sampled.

- Given correlation matrix is not positive definite.

- Certain correlations do not satisfy (3.2) or (3.3). In this case (3.1) is not applied to compute correlations $\mathrm{cor}\,(\widetilde{x}_i, \widetilde{x}_j)$, but original correlations $\mathrm{cor}\,(\widetilde{x}_i, \widetilde{x}_j) = \mathrm{cor}\,(x_i, x_j)$ are used instead. ENDSAM gives the number and the list of such correlations.

- Correlation matrix $[\mathrm{cor}\,(\widetilde{x}_i, \widetilde{x}_j)]$ is not positive definite. In this case its nearest correlation matrix is computed. ENDSAM gives the number of nonpositive eigenvalues and the smallest eigenvalue.

We have tested ENDSAM by processing files from three major nuclear data labraries: ENDF/B-VII.1 [3], JEFF 3.2 [4], and JENDL 4.0 [5]. In these libraries, we spotted all the inconsistencies which are listed above. However, we did not find any of the possible inconsistencies which follow, but the program would catch them in order to avoid problems with reading data or computations.

ENDSAM throws an error and moves to the next file on the list if any of the following inconsistencies occurs.

- A certain correlation between resonance parameters has a value which is not between -1 and 1.

- Flags EL and EH do not satisfy 0<EL<EH.

- A certain energy range from File 32 was not found in File 2. Energy ranges are considered to agree if the values of EL agree up to a relative error of $10^{-3}\%$ and EH is smaller or equal in File 32 up to the same relative error.

- Corresponding energy ranges from File 2 and File 32 do not have consistent values of flags LRU or LRF.

- The name of ENDF file is longer than '149 minus number of digits of number of samples' characters.

- File with a name from the list in input file was not found.

ENDSAM throws an error and aborts the execution if any of the following occurs. Except for the first one, they are not inconsistencies of the library.

- Certain values of flags appear which are not valid in ENDF-6 format.

- Combinations of values of flags occur which are valid, but not implements yet:
  - NIS > 1
  - LRU=1 and LRF=4
  - MF=2 and LRU=1 and LRF=7 and KBK$\neq$0 or KPS$\neq$0 or KRM$\neq$3
  - MF=2 and LRU=2 and LRF=1
  - MF=32 and LRU=1 and NRO=1
  - MF=32 and LRU = 1 and LRF=1or2or3 and LCOMP = 1 and NLRS>0.

- Number of samples is set to be negative.

- Iteration in Higham's method to find nearest correlation matrix does not converge.

5 Output: files in ENDF-6 format

In this section we give an example of input and output file in ENDF-6 format. We process the file of isotope ^{23}Na from ENDF/B-VII.1 library. File 2 is the following.

```
1.102300+4 2.279200+1          0          0          1          01125 2151    1
1.102300+4 1.000000+0          0          0          1          01125 2151    2
6.000000+2 5.000000+5          1          2          0          01125 2151    3
1.500000+0 5.410000-1          0          0          3          01125 2151    4
2.279200+1 0.000000+0          0          0         24         41125 2151    5
2.810000+3 1.000000+0 3.763400+2 3.760000+2 3.530000-1 0.000000+01125 2151    6
2.429700+5 1.000000+0 3.295000+2 3.280000+2 1.500000+0 0.000000+01125 2151    7
2.983200+5 2.000000+0 2.039000+3 2.038000+3 1.020000+0 0.000000+01125 2151    8
5.385700+5 1.000000+0 6.278000+4 6.277000+4 1.014000+1 0.000000+01125 2151    9
2.279200+1 0.000000+0          1          0         72        121125 2151   10
7.617000+3 2.000000+0 6.058000-1 5.800000-3 6.000000-1 0.000000+01125 2151   11
3.539000+4 1.000000+0 3.500000+0 1.600000+0 1.900000+0 0.000000+01125 2151   12
5.322000+4 2.000000+0 1.112800+3 1.112000+3 7.850000-1 0.000000+01125 2151   13
1.174300+5 1.000000+0 3.103000+1 2.680000+1 4.230000+0 0.000000+01125 2151   14
1.431300+5 0.000000+0 2.360000+1 1.650000+1 7.100000+0 0.000000+01125 2151   15
2.011500+5 1.000000+0 4.927900+3 4.925000+3 2.940000+0 0.000000+01125 2151   16
2.143000+5 0.000000+0 1.428500+4 1.428000+4 4.640000+0 0.000000+01125 2151   17
2.390500+5 2.000000+0 5.350200+3 5.349000+3 1.200000+0 0.000000+01125 2151   18
2.994100+5 1.000000+0 1.325600+2 1.300000+2 2.560000+0 0.000000+01125 2151   19
3.923200+5 1.000000+0 2.277000+4 2.276000+4 9.870000+0 0.000000+01125 2151   20
5.980000+5 1.000000+0 2.580000+4 2.580000+4 0.000000+0 0.000000+01125 2151   21
7.270000+5 3.000000+0 4.500000+4 4.500000+4 0.000000+0 0.000000+01125 2151   22
2.279200+1 0.000000+0          2          0         42         71125 2151   23
1.900600+5 0.000000+0 2.750000+1 1.820000+1 9.300000+0 0.000000+01125 2151   24
2.367100+5 2.000000+0 6.679000+1 6.520000+1 1.590000+0 0.000000+01125 2151   25
3.052000+5 0.000000+0 7.800000+1 6.830000+1 9.700000+0 0.000000+01125 2151   26
4.309000+5 0.000000+0 4.005300+3 4.000000+3 5.290000+0 0.000000+01125 2151   27
4.488200+5 2.000000+0 7.029500+3 7.026000+3 3.520000+0 0.000000+01125 2151   28
6.970000+5 4.000000+0 6.000000+4 6.000000+4 0.000000+0 0.000000+01125 2151   29
7.800000+5 4.000000+0 4.400000+4 4.400000+4 0.000000+0 0.000000+01125 2151   30
0.000000+0 0.000000+0          0          0          0          01125 2  099999
```

After reading this file, ENDSAM lets us know that there are 23 resonances in File 2. Indeed, they appear in the lines $6 - 9$, $11 - 22$, and $24 - 30$.

```
1.102300+4 2.279200+1          0          0          1          0112532151    1
1.102300+4 1.000000+0          0          0          1          0112532151    2
6.000000+2 5.000000+5          1          2          0          0112532151    3
1.500000+0 5.410000-1          0          2          0          0112532151    4
2.279200+1 0.000000+0          0          0        276         23112532151    5
2.810000+3 1.000000+0 3.763400+2 3.760000+2 3.530000-1 0.000000+0112532151    6
4.013280+0 0.000000+0 0.000000+0 6.998690+0 6.800100-3 0.000000+0112532151    7
7.617000+3 2.000000+0 6.058000-1 5.800000-3 6.000000-1 0.000000+0112532151    8
```

```
1.142550+1 0.000000+0 0.000000+0 4.640000-4 6.000000-2 0.000000+0112532151    9
3.539000+4 1.000000+0 3.500000+0 1.600000+0 1.900000+0 0.000000+0112532151   10
2.117700+0 0.000000+0 0.000000+0 1.730000-1 2.100000-1 0.000000+0112532151   11
5.322000+4 2.000000+0 1.112800+3 1.112000+3 7.850000-1 0.000000+0112532151   12
4.979462+1 0.000000+0 0.000000+0 3.500280+1 7.800000-2 0.000000+0112532151   13
1.174300+5 1.000000+0 3.103000+1 2.680000+1 4.230000+0 0.000000+0112532151   14
1.100659+2 0.000000+0 0.000000+0 1.145000+1 7.100000-1 0.000000+0112532151   15
1.431300+5 0.000000+0 2.360000+1 1.650000+1 7.100000+0 0.000000+0112532151   16
1.402086+2 0.000000+0 0.000000+0 2.250000+0 4.900000-1 0.000000+0112532151   17
1.900600+5 0.000000+0 2.750000+1 1.820000+1 9.300000+0 0.000000+0112532151   18
1.901000+2 0.000000+0 0.000000+0 5.216000+0 1.268000+0 0.000000+0112532151   19
2.011500+5 1.000000+0 4.927900+3 4.925000+3 2.940000+0 0.000000+0112532151   20
2.010000+2 0.000000+0 0.000000+0 3.760036+2 9.550000-1 0.000000+0112532151   21
2.143000+5 0.000000+0 1.428500+4 1.428000+4 4.640000+0 0.000000+0112532151   22
2.093280+2 0.000000+0 0.000000+0 8.867000+2 7.600000-1 0.000000+0112532151   23
2.367100+5 2.000000+0 6.679000+1 6.520000+1 1.590000+0 0.000000+0112532151   24
2.391377+2 0.000000+0 0.000000+0 1.210000+1 3.000000-1 0.000000+0112532151   25
2.390500+5 2.000000+0 5.350200+3 5.349000+3 1.200000+0 0.000000+0112532151   26
2.391500+2 0.000000+0 0.000000+0 9.980000+1 2.060020-1 0.000000+0112532151   27
2.429700+5 1.000000+0 3.295000+2 3.280000+2 1.500000+0 0.000000+0112532151   28
2.405601+2 0.000000+0 0.000000+0 1.620000+1 4.130000-1 0.000000+0112532151   29
2.983200+5 2.000000+0 2.039000+3 2.038000+3 1.020000+0 0.000000+0112532151   30
2.986500+2 0.000000+0 0.000000+0 4.875000+1 1.342000-1 0.000000+0112532151   31
2.994100+5 1.000000+0 1.325600+2 1.300000+2 2.560000+0 0.000000+0112532151   32
2.995400+2 0.000000+0 0.000000+0 6.724000+0 4.270000-1 0.000000+0112532151   33
3.052000+5 0.000000+0 7.800000+1 6.830000+1 9.700000+0 0.000000+0112532151   34
2.993018+2 0.000000+0 0.000000+0 9.820000+0 1.940000+0 0.000000+0112532151   35
3.923200+5 1.000000+0 2.277000+4 2.276000+4 9.870000+0 0.000000+0112532151   36
3.909906+2 0.000000+0 0.000000+0 2.276000-1 2.700037+0 0.000000+0112532151   37
4.309000+5 0.000000+0 4.005300+3 4.000000+3 5.290000+0 0.000000+0112532151   38
4.315300+2 0.000000+0 0.000000+0 6.780000+2 6.970000-1 0.000000+0112532151   39
4.488200+5 2.000000+0 7.029500+3 7.026000+3 3.520000+0 0.000000+0112532151   40
4.497200+2 0.000000+0 0.000000+0 1.400000-1 5.860140-1 0.000000+0112532151   41
5.385700+5 1.000000+0 6.278000+4 6.277000+4 1.014000+1 0.000000+0112532151   42
4.411600+2 0.000000+0 0.000000+0 4.135000+4 2.000014+0 0.000000+0112532151   43
5.980000+5 1.000000+0 2.580000+4 2.580000+4 0.000000+0 0.000000+0112532151   44
2.990000+3 0.000000+0 0.000000+0 3.800048+3 0.000000+0 0.000000+0112532151   45
6.970000+5 4.000000+0 6.000000+4 6.000000+4 0.000000+0 0.000000+0112532151   46
3.418000+3 0.000000+0 0.000000+0 9.600000+3 0.000000+0 0.000000+0112532151   47
7.270000+5 3.000000+0 4.500000+4 4.500000+4 0.000000+0 0.000000+0112532151   48
3.598613+3 0.000000+0 0.000000+0 7.200000+3 0.000000+0 0.000000+0112532151   49
7.800000+5 4.000000+0 4.400000+4 4.400000+4 0.000000+0 0.000000+0112532151   50
3.888800+3 0.000000+0 0.000000+0 7.040000+3 0.000000+0 0.000000+0112532151   51
0.000000+0 0.000000+0          3         69          0          0112532151   52
0.000000+0 0.000000+0          0          0          0          0112532  099999
```

Here, ENDSAM returns that there are 69 resonance parameters with covariance data, out of which 65 are nonconstant. Indeed, their mean values appear in columns 1, 4, and 5

of even lines from 6 to 50, while their deviations appear one line below mean values. Zero deviations of parameters with covariance data thus appear in column 5 of lines 45, 47, 49, and 51.

Next, ENDSAM informs us that correlation matrix equals identity matrix which can be seen from zero value in column 5 of line 52.

The next step is to make random samples and in the end their values are written to new files in ENDF-6 format. If original file has the name File.ext and n is the number of samples, then sampled files have names File_1.ext, . . . , File_n.ext. Below we give an example of File 2 which contains sampled values.

```
1.102300+4 2.279200+1          0          0          1          01125 2151    1
1.102300+4 1.000000+0          0          0          1          01125 2151    2
6.000000+2 5.000000+5          1          2          0          01125 2151    3
1.500000+0 5.410000-1          0          0          3          01125 2151    4
2.279200+1 0.000000+0          0          0         24          41125 2151    5
2.811069+3 1.000000+0 3.763400+2 3.704244+2 3.664647-1 0.000000+01125 2151    6
2.428422+5 1.000000+0 3.295000+2 3.225574+2 1.605526+0 0.000000+01125 2151    7
2.980303+5 2.000000+0 2.039000+3 2.024915+3 8.057385-1 0.000000+01125 2151    8
5.379616+5 1.000000+0 6.278000+4 6.362465+4 8.786140+0 0.000000+01125 2151    9
2.279200+1 0.000000+0          1          0         72         121125 2151   10
7.612944+3 2.000000+0 6.058000-1 5.523922-3 5.520258-1 0.000000+01125 2151   11
3.538575+4 1.000000+0 3.500000+0 1.583915+0 1.795089+0 0.000000+01125 2151   12
5.324757+4 2.000000+0 1.112800+3 1.143244+3 6.466060-1 0.000000+01125 2151   13
1.175479+5 1.000000+0 3.103000+1 3.865670+1 3.165214+0 0.000000+01125 2151   14
1.429167+5 0.000000+0 2.360000+1 1.616699+1 6.442193+0 0.000000+01125 2151   15
2.014819+5 1.000000+0 4.927900+3 5.062836+3 3.339159+0 0.000000+01125 2151   16
2.142452+5 0.000000+0 1.428500+4 1.510002+4 4.793710+0 0.000000+01125 2151   17
2.391225+5 2.000000+0 5.350200+3 5.387397+3 1.256445+0 0.000000+01125 2151   18
2.992458+5 1.000000+0 1.325600+2 1.224137+2 2.427136+0 0.000000+01125 2151   19
3.924053+5 1.000000+0 2.277000+4 2.275973+4 1.304718+1 0.000000+01125 2151   20
5.992946+5 1.000000+0 2.580000+4 3.042950+4 0.000000+0 0.000000+01125 2151   21
7.312937+5 3.000000+0 4.500000+4 3.938414+4 0.000000+0 0.000000+01125 2151   22
2.279200+1 0.000000+0          2          0         42          71125 2151   23
1.900883+5 0.000000+0 2.750000+1 2.167164+1 1.024670+1 0.000000+01125 2151   24
2.365003+5 2.000000+0 6.679000+1 8.986865+1 1.741793+0 0.000000+01125 2151   25
3.052484+5 0.000000+0 7.800000+1 6.933420+1 1.021129+1 0.000000+01125 2151   26
4.308275+5 0.000000+0 4.005300+3 4.092822+3 5.787986+0 0.000000+01125 2151   27
4.488591+5 2.000000+0 7.029500+3 7.026158+3 3.618211+0 0.000000+01125 2151   28
6.914366+5 4.000000+0 6.000000+4 7.335487+4 0.000000+0 0.000000+01125 2151   29
7.823972+5 4.000000+0 4.400000+4 5.083665+4 0.000000+0 0.000000+01125 2151   30
0.000000+0 0.000000+0          0          0          0          01125 2  099999
```

References

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