ENSDF Analysis and Checking Codes

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June 29, 1993

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1 General

This document describes the current status of the ENSDF analysis and checking codes available from the National Nuclear Data Center (NNDC), their availability for VAX/VMS, ANSI, or MS-DOS, methods of obtaining the codes and associated information, and some recent changes. Tables 1-2 summarize the current status; section 2 outlines how to obtain the VAX/VMS and ANSI versions from the NNDC VAX-cluster; and section 3 provides details on the contents and how to obtain the MS-DOS versions. Appendix A has some notes which may be of interest to programmers.

1.1 Major Enhancements Since August 1992

FMTCHK

1. Spurious messages eliminated.
2. Summary of number of messages displayed on terminal.
3. Check order of level energies.
4. Check for valid data set identification on X records.
5. More syntax checking on N and PN records and cross checking between N and PN record and fields.
6. More checking on the identification record.
7. Added documentation on the warning and error messages to the "Read me" file READFMTC.ME.
8. Finished implementation of update (U) comment.

GTOL

1. Compact symmetric matrix inversion reduces memory requirements.
2. First level encountered is always assumed to be fixed.
3. Non-numeric level energies of the form "num+X", *etc.* are properly handled.
4. Non-numeric level energies of the form "SP+num" are ignored.
5. Production normalization (PN) record implemented.
6. Non-numeric uncertainties on feeding radiations retained for output.

7. "FL=" updated when new file created.
8. Size of report reduced.

1.2 Substantive Changes Since August 1992

HSICC

1. Publication comment coding added in version 11(6) replaced with coding to put CC on "S G" record.
2. Improved logic on handling uncertainties.
3. Improved logic on number of significant digits to retain in output.

LOGFT

1. More terminal output warning of possible problems.
2. Faster integration routines added.
3. Production normalization record implemented.
4. More checking on input data.

1.3 Codes Added to the Distribution Since August 1992

ALPHAD ALPHAD calculates α-hindrance factors. The program was provided by the Nuclear Data Project.

ENSDAT ENSDAT creates tables and drawings from ENSDF-formatted files in a form similar to the Nuclear Data Sheets.

GABSPC This program has been received from Coral Baglin and is the MS-DOS version of the program GABS.

1.4 Data Library Changes

LOGFT.DAT Data were corrected for $Z \leq 4$ in April 1989 corresponding to changes made in version 7(1) of LOGFT.

1.5 "Read Me" Files

All program packages now have an associated "Read Me" file. These files include a basic description of the program, how to compile and run the program, the version history, and current group responsible for the program. For programs with no published documentation, additional details are given in the "Read Me."[1]

[1] Where possible, unpublished documentation is provided as a file with the distribution.

Table 1: Status of ENSDF Analysis and Checking Codes (June 24, 1993)

Code	Function	Version[a] No./Date	MS-DOS	Documentation
ADDGAM	Adds γ's to adopted data set.	1(3) 930414	Yes	No (See "Read Me" file)
ALPHAD	Calculates α HF's and theoretical $T^{\alpha}_{\frac{1}{2}}$'s	1.2 930421	Yes	No (See "Read Me" file)
DELTA	Analyzes angular correlation data.	1.01 930415	Yes	LUNFD/(NFFR-3048) 1-27
ENSDAT	Produces tables and drawings	3.23[b] 930624	Yes	No (See "Read Me" file)
FMTCHK	ENSDF format checking.	8.1a 930513	Yes	No (See "Read Me" file)
GABS	Calculates absolute ΔI_{γ}'s.	V[c] 8902	No	Yes
GABSPC		9109	Yes	
GAMUT	Creates adopted levels, gammas from source data sets.	[c,d] 8809	No	LBL-26024
GTOL	Determines level energies from a least-squares fit to E_{γ}'s & feedings.	6.0 930407	Yes	BNL-NCS-23375/R LUNFD/(NFFR-3049) 1-27
HSICC	Interpolates internal conversion coefficients.	11(9) 920909	Yes	Nucl. Data A4, 1 Nuclear Data Tables A9, 119 BNL-NCS-23375/R
LOGFT	Calculates log ft.	7(12) 930510	Yes	Nucl. Data Tables A10, 206
NSDFLIB	Support subprograms for many codes	4(12) 930401	Yes	Yes
PANDORA	Physics check of ENSDF data sets. Aids with adopted gammas & XREF.	5(8) 930526	Yes	Yes
PREND	Constructs level schemes from ENSDF data sets.	2.4[d] 9101	No	Yes

[a]Please check with the NNDC as to more recent versions.
[b]MS-DOS only.
[c]Program as received from the author.
[d]Program contains VAX extensions of ANSI-standard FORTRAN 77.

Table 2: Status of ENSDF Analysis and Checking Codes (June 24, 1993) (Continued)

Code	Function	Version[a] No./Date	MS-DOS	Documentation
RADLST	Calculates atomic & nuclear radiations. Checks energy balance.	5.4g 880321	No	BNL-NCS-52142
RULER	Calculates reduced transition probabilities.	1.16 930524	Yes	Yes
SPINOZA	Physics check of an ENSDF data set.	1(2) 871102	No	Yes
TREND	Tabular display of ENSDF data.	6.13a 930519	Yes	No (See "Read Me" file)

2 On-line Access

VAX and ANSI-standard source codes, relevant documentation, data, and sample input and output may be obtained directly from the NNDC VAX cluster either through the NNDC Online Data Service or by direct retrieval from an anonymous account using FTP. The programs may also be obtained in other media on request (see page 8 for the address); however, there may be a delay in satisfying such requests.

2.1 NNDC Online Data Service

After logging on to the NNDC Online Data Service, select the FILES/CODES option. Within the CODES menu, select either ENSDF_UTILITY[2] or ENSDF_ANALYSIS[3] and then select either ANSI-77 for source code conforming to ANSI FORTRAN 77 or VAX/VMS for source code which may contain VAX/VMS FORTRAN 77 extensions.[4] After selecting the desired programs or documentation, the user will be queried as to the method of file transmission. The selected programs along with relevant documentation, data files, and subprogram libraries will be then transmitted *via* the selected method.

Note that if the user selects DOCUMENTATION, the file DISTRM.MEM will be transmitted. This file contains a table listing the latest version numbers and dates of the programs. It also contains brief descriptions of each code, machine dependencies and availability, data required, and subprogram library dependencies.

2.2 Anonymous Account

The ENSDF codes, documentation, and data may also be obtained by logging into an anonymous account[5] using FTP. A sample dialog would be:

[2] General documentation, NSDFLIB, ADDGAM, FMTCHK, PREND, and TREND

[3] General documentation, NSDFLIB, DELTA, GABS, GAMUT, GTOL, HSICC, LOGFT, PANDORA, RADLST, RULER, and SPINOZA

[4] Please use the Data Service HELP feature to obtain more details.

[5] Directory restrictions apply.

```
ftp bnlnd2.dne.bnl.gov
Name: bnlndc
Password:
ftp>get [scr.ensdf_pgm]readme.1st
ftp>bye
```

This will connect the user to the NNDC anonymous account, log into the anonymous account, retrieve the file README.1ST,[6] and disconnect. Figure 1 outlines the current organization of the directory. General information, data, and FORTRAN sources are contained in ENSDF_PGM and all relevant files for each program are contained in a subdirectory with the program name.

The file DISTRM.MEM in ENSDF_PGM contains a table listing the latest version numbers and dates of the programs. It also contains brief descriptions of each code, machine dependencies and availability, data required, and subprogram library dependencies. Each subdirectory contains a "Read me" file (*e.g.*, READADDG.ME in ADDGAM) which provides additional details about the program.

Extensions for the FORTRAN source codes follow the following conventions:

ANS ANSI-standard FORTRAN 77 code with machine-dependent coding included.[7]

FOR ANSI-standard FORTRAN 77 code with no machine-dependent coding included.

VAX FORTRAN 77 code with VAX/VMS extensions and, possibly, machine-dependent coding.[7]

Other machine-dependent source codes (*e.g.*, for IBM PC's and clones) may be constructed by downloading the ANSI version of the code and the program SETMDC found in the ENSDF_PGM directory.

3 MS-DOS Distribution

A distribution of MS-DOS versions has been prepared. It includes all of the ENSDF analysis and checking codes[8] except for GAMUT, PREND, RADLST, and SPINOZA.[9] In addition to the FORTRAN source code, sample input and output, and documentation, this distribution also contains the executable code and object libraries, installation batch files, and installation notes. The standard distribution consists of four $3\frac{1}{2}$-inch high-density diskettes.[10]

The distribution may be requested by either leaving a note on the NNDC Online Data Service or by contacting:

[6] Contains the current information on the organization and content of the ENSDF analysis and checking codes directory ENSDF_PGM

[7] Machine-dependent coding is in the form of special comments recognized by the program SETMDC.

[8] All MS-DOS versions are current with VAX/VMS and ANSI versions as of June 24, 1993.

[9] The program GABSPC has been substituted for GABS and the program ENSDAT is included in this distribution.

[10] Other media can be specified but there may be a delay in satisfying the request.

Figure 1: NNDC ENSDF Program Directory Tree

```
ENSDF_PGM
    |
    |-----ANALYSIS
    |        |
    |        |-----ALPHAD
    |        |-----DELTA
    |        |-----GABS
    |        |-----GAMUT
    |        |-----GTOL
    |        |-----HSICC
    |        |-----LOGFT
    |        |-----PANDOR
    |        |-----RADLST
    |        |-----RULER
    |        |-----SPINOZ
    |
    |-----DATA.TST
    |-----DISTRM.MEM
    |-----NSDFLIB.FOR
    |-----NSDFLIB.MEM
    |-----README.1ST
    |-----READNSDF.ME
    |-----SETMDC.ANS
    |-----SETMDC.MEM
    |-----SETMDC.VAX
    |
    |-----UTILITY
    |        |
    |        |-----ADDGAM
    |        |-----FMTCHK
    |        |-----PREND
    |        |-----TREND
```

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4 Reporting Problems

If problems occur in using the ENSDF analysis and checking codes, please check the version of the program you are using. If you are not using the current version (see Table 1), please obtain the latest version (See sections 2 and 3). If the problem is in the latest version of the program, please contact the authors listed in the associated "Read me" file and include in your report the input data, a description of the problem, and the version number of the program. If you are unable to contact the author, please send the report to the NNDC.[11]

5 Disclaimer

Neither the Associated Universities, Inc., nor the US Department of Energy make any warranty or assume any legal responsibility for the results produced by the programs and data included in this distribution.

A Notes to Programmers

In preparing the MS-DOS distribution several compiler-related problems were noted which may be of interest.

A.1 Intermediate Storage of Calculations

While there are ANSI and IEEE standards for the storage of REAL (4 byte) and DOUBLE PRECISION (8 byte) numbers, some compilers default to storing intermediate values in a machine register until all calculations required for a variable's final value are completed.[12] This is usually done in the interest of reducing roundoff error, code size, and, presumably, processing time. However, this may result in differences when comparing outputs on different machines (Likely candidates are GAMUT and GTOL with their least-squares fitting, GTOL in the summing of I_γ's, and LOGFT in the integrations to obtain $\log ft$, I_β, I_ϵ, and $<E_\beta>$).[13]

[11] See page 8.
[12] Microsoft Optimizing FORTRAN 5.0 uses an 80-bit machine register.
[13] VAX/VMS FORTRAN appears to store the intermediate results in the variable.

A.2 Implicit Casting of Variables

Another problem may occur when there is an implicit cast of variables (*e.g.*, REAL to DOUBLE PRECISION). Different compilers seem to do the casting differently. The following simple code:

```
      Real x,z
      Double Precision y
C
      Double Precision DBLE
      Intrinsic DBLE
C
      z=100.
      x=10.**(-10)
      y=z+x
      Write(*,*)'z+x=',y
      y=z+x
      Write(*,*)'DBLE(z+x)=',y
      y=DBLE(z)+DBLE(x)
      Write(*,*)'DBLE(z)+DBLE(x)=',y
      End
```

produced the following results when compiled and run on a VAX 11/8820:

```
z+x=   100.0000000000000
DBLE(z+x)=   100.0000000000000
DBLE(z)+DBLE(x)=   100.0000000001000
```

When the same code was run on a 386DX/25 using Microsoft Optimizing FORTRAN 5.0 with the `/Op` switch in compilation to avoid the problem discussed in section A.1, the results were:

```
z+x=     100.000000000100000
DBLE(z+x)=     100.000000000100000
DBLE(z)+DBLE(x)=     100.000000000100000
```

It appears that VAX/VMS FORTRAN does not cast until after the operation and Microsoft FORTRAN casts before the operation. This does not appear to have any significant effects in the current codes.

A.3 Definition of Double Precision

There appears to be different interpretations of DOUBLE PRECISION. In VAX/VMS FORTRAN, the default DOUBLE PRECISION variable may have an absolute value between $\approx 0.29 \times 10^{-38}$ and $\approx 1.7 \times 10^{+38}$ with about 16 significant digits. A DOUBLE PRECISION variable in Microsoft FORTRAN 5.0 may have an absolute value between $\approx 2.2 \times 10^{-308}$ and $\approx 1.8 \times 10^{+308}$ with about 15 significant digits; this is roughly equivalent but not identical to the VAX/VMS range ($\approx 0.56 \times 10^{-308}$ to $\approx 0.9 \times 10^{+308}$) when the

G_FLOATING option is used during compilation. This affected the code DELTA where, among other large numbers, $56! = 7.11 \times 10^{+74}$ was calculated.[14]

[14] The code was modified to conform to the minimum default definition.