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16-APR-03 Final Release of ENDF/B-V for use with LLNL Codes

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The Computational Nuclear Physics Group in N Division is issuing the first official release of the ENDF/B-V evaluations for users of **ndf**, **mcf** and **TART** data files. The new files can be found on OCF (blue and compass) and SCF (sky and forest) in the appropriate subdirectories of

/usr/gapps/data/nuclear/endfb5/endfb5r2
and
/usr/gapps/data/nuclear/endfb5/endfb5r2+endl99.

These data files are in Cray binary format. The **pdb** versions of the **mcf** data have also been prepared for **CMCAPM** users (fortran version unsupported).

The new data files were prepared in two steps. First, the ENDF/B-V database was translated to an ENDL-format ascii database. The ENDL ascii format is a point-wise tabular storage scheme where intermediate values are extracted via interpolation. Sufficient point-wise information was generated in the translation to insure an extraction tolerance of 0.1% for most of the data. The only exception is along the incident neutron energy axis of the outgoing particle energy probability density function where a 0.5% tolerance was maintained. Second, processed files were generated from the translated database. Since the translated ENDF/B-V data is in ENDL-format, the standard processing codes were used to generate the new processed data files. To the best of our knowledge, these processed data files are accurate representations of the ENDF/B-V database to within the stated tolerances. However, there are several issues that users must be aware of:

1. The ENDF/B-V database does not contain a carbon 12 evaluation. After the translation, a copy of the natural carbon evaluation (za006000) was added and renamed carbon 12 (za006012). The carbon 12 file was added to enhance compatibility since the ENDL database does not contain natural carbon. Technically, this is acceptable since natural carbon is 98.9% carbon 12.

2. The format of the ENDF/B-V database severely limits the amount of information that can be stored about outgoing charged particles. Cross sections with exit channels containing charged particles are numerous; however, outgoing charged particle energy and angular distributions are not. As part of the processing, we determine the "missing" charged particle energy from kinematics and deposit it locally.

3. The ENDF/B-V gamma-ray production information is often not associated with particular exit channels. Instead, the (n,Xgamma) channel is used to store the gamma-rays which are not explicitly associated with particular reactions. Summing the gamma-ray production channels in order to determine a single gamma-ray source term for each isotope will produce the desired result.

4. The format of the ENDF/B-V database provides no means of storing double differential data. Therefore, the angular and energy information of outgoing particles is completely uncorrelated.

5. There are 110 targets in ENDL94/ENDL99 and 124 in ENDF/B-V; only 68 of them are common to both databases. The lists of targets are presented below in order of atomic number (Z*1000) plus mass number (A). The common targets are in bold print.

ENDL94 Targets

za000001 **za001001 za001002 za001003 za002003 za002004 za003006 za003007** za004007 **za004009 za005010 za005011** za006012 za006013 **za007014 za007015 za008016 za009019** za010020 **za011023 za012000 za013027 za014000 za015031 za016032 za017000** za018000 **za019000 za020000 za022000** za023051 **za024000 za025055 za026000 za027059 za028000** za028058 **za029000** za030000 **za031000** za033074 za033075 za039088 za039089 **za040000 za041093 za042000 za047107 za047109 za048000** za049000 za050000 za051000 za053127 za054000 **za054134 za056138 za063000** za064000 za067165 **za072000 za073181 za074000 za075185 za075187** za078000 **za079197** za080000 **za082000 za083209** za090231 **za090232** za090233 **za091233 za092233 za092234 za092235 za092236** za092237 **za092238** za092239 za092240 za093235 za093236 **za093237** za093238 za094237 **za094238 za094239 za094240 za094241 za094242** za094243 **za095241 za095242m za095243** za096242 **za096243 za096244 za096245 za096246** za096247 za096248 za097249 za098249 za098250 za098251 za098252 za099120 za099125

ENDF/B-V Targets

za001001 za001002 za001003 za002003 za002004 za003006 za003007 za004009 za005010 za005011 za006000 **za007014 za007015 za008016** za008017 **za009019 za011023 za012000 za013027 za014000 za015031** za016000 **za016032 za017000 za019000 za020000 za022000** za023000 **za024000 za025055 za026000 za027059 za028000 za029000 za031000** za036078 za036080 za036082 za036083 za036084 za036086 za037085 za037087 **za040000** za040090 za040091 za040092 za040094 za040096 **za041093 za042000** za043099 za045103 **za047107 za047109 za048000** za048113 za054124 za054126 za054128 za054129 za054130 za054131 za054132 **za054134** za054135 za054136 za055133 **za056138** za062149 **za063000** za063151 za063152 za063153 za063154 za064152 za064154 za064155 za064156 za064157 za064158 za064160 za066164 za071175 za071176 **za072000** za072174 za072176 za072177 za072178 za072179 za072180 **za073181** za073182 **za074000** za074182 za074183 za074184 za074186 **za075185 za075187 za079197 za082000 za083209 za090232 za091233 za092233 za092234 za092235 za092236 za092238 za093237 za094238 za094239 za094240 za094241 za094242 za095241 za095242m za095243 za096243 za096244 za096245 za096246** za099121 za099122

6. In addition to the target inventory of ENDF/B-V, we have included the two fission fragment files generated and used at Los Alamos. These fission fragment files, listed as za099121 and za099122, are "typical" fission fragments for uranium (za045117) and plutonium (za046119). These files are an average over evaluations performed for the ten most common fission fragments for each actinide.

7. Many of the ENDF/B-V evaluations have no gamma-ray information. For these 66 evaluations we add an (n,Xgamma) cross section which is zero over the entire incident neutron energy range. The presence of these null files insures that these isotopes are listed in the photon production libraries. As a result, users can choose to track photons without modifying their assemblies or codes. Below is the list of evaluations which have no gamma-ray information:

za001003 za002003 za002004 za005011 za008017 za036078 za036080 za036082
za036083 za036084 za036086 za037085 za037087 za040000 za040090 za040091
za040092 za040094 za040096 za043099 za045103 za047107 za047109 za048000
za048113 za054124 za054126 za054128 za054129 za054130 za054131 za054132
za054134 za054135 za054136 za055133 za062149 za063000 za063152 za063154
za064152 za064154 za064155 za064156 za064157 za064158 za064160 za066164
za071175 za071176 za072000 za072174 za072176 za072177 za072178 za072179
za072180 za073182 za075185 za075187 za079197 za091233 za092234 za092236
za093237 za094238

8. The ENDF/B-V database contains only neutron-induced reactions and therefore only those data files were processed. Below is a listing of the new files residing in the **endfb5r2** directory:

Directory structure	Description
mcf/	**mcf** data sub-directory
mcf1	neutron data
mcf1.pdb	neutron data (pdb format)
ndf/	**ndf** data sub-directory
ndf1.087	87 group neutron data (bdfls id=4)
ndf1.175	175 group neutron data (bdfls id=6)
ndf1.230	230 group neutron data (bdfls id=7)
tart/	**TART** data sub-directory
tartppd	175 group photon production data
tartnd	175 group neutron interaction data
cross	type-2 banding data

File	Date	sha output (i.e., checksum)
mcf/mcf1	030301	`a0647968 359eb35e b253b4d3 ea1aa0ef c877990a`
mcf/mcf1.pdb	030302	`1e6606a4 a32b7b51 536d86ed 9fdfce3c d9e3723d`
ndf/ndf1.087	030303	`4a7bf261 aebdaa1b dd93d254 25ea49a3 91003d30`
ndf/ndf1.175	030304	`30960a2b cf7c5a21 9b6e15c4 4d8cb070 5a6732ce`
ndf/ndf1.230	030305	`e5d69525 51199d62 c4fcc0a2 b37af053 9d8b6122`
tart/tartppd	030309	`198ff812 f873784d 0cc60c60 2928ad6d b20ffccc`
tart/tartnd	030308	`169ab7c8 b1eb3171 fa6c74e9 eb7d9d59 335e2c64`
tart/cross	030306	`82b4ae70 e6204cdc 156b48ab 7bc9cc92 fb94428a`

9. We anticipate that some users and code developers may wish/need to avoid modifying assembly compositions due to missing evaluations in the ENDF/B-V data. For these users we have constructed a hybrid library which contains the ENDF/B-V evaluations and the unique ENDL evaluations. This hybrid library allows user codes to run without modification to their assembly and gain access to the ENDF/B-V data when it is available. Below is a listing of the new files residing in the **endfb5r2+endl99** directory:

Directory structure	Description
mcf/	**mcf** data sub-directory
mcf1	neutron data
mcf1.pdb	neutron data (pdb format)
ndf/	**ndf** data sub-directory
ndf1.087	87 group neutron data (bdfls id=4)
ndf1.175	175 group neutron data (bdfls id=6)
ndf1.230	230 group neutron data (bdfls id=7)
tart/	**TART** data sub-directory
tartppd	175 group photon production data
tartnd	175 group neutron production data
cross	type-2 banding data

File	Date	sha output (i.e., checksum)
mcf/mcf1	030310	3ba67041 8dc94a53 1214b405 cf4d0177 e86fa5fc
mcf/mcf1.pdb	030311	7ffa68d0 a4fe4491 c9261b02 386323e1 353c6528
ndf/ndf1.087	030312	7b68d488 6508eb31 67eb5600 c2d74ebb 05db7263
ndf/ndf1.175	030313	24e93be6 90ce813b 15163cd6 c50cb82c cc4fd05f
ndf/ndf1.230	030314	43c49438 fba7e8de b65fe19e 2501c334 5c3f786e
tart/tartppd	030317	8464defb 8dc10504 c3e0d360 dfa9f4e3 cfc98019
tart/tartnd	030316	2c1a1032 8d6ce60f 041e6af6 0afb6f0d 0da96607
tart/cross	030315	2f466985 42cef6d1 e122d720 33ef3c4e 54eb1aed

Testing has been carried out using a variety of LLNL codes to insure basic compatibility. However, given the limited information present in the ENDF/B-V database, some client codes may not run in the "standard" mode and users need to carefully consider the issues listed above.

Last but not least, the Computational Nuclear Physics Group would like to thank D.E. Cullen and D.A. Resler