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The new ENSDF search system NESSY: IBM/PC nuclear spectroscopy database

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Abstract

The universal relational nuclear structure and decay database NESSY (New ENSDF Search SYstem) developed for the IBM/PC and compatible PCs, and based on the international file ENSDF (Evaluated Nuclear Structure Data File), is described. The NESSY provides the possibility of high efficiency processing (the search and retrieval of any kind of physical data) of the information from ENSDF. The principles of the database development are described and examples of applications are presented.

1. Introduction

The Evaluated Nuclear Structure Data File (ENSDF) [1] now contains data for all known nuclides. ENSDF is produced and supported by IAEA international cooperation with the main responsibility lying with the USA BNL National Nuclear Data Center, and is regularly updated. The main emphasis in ENSDF preparation is on experimental information: only well known and reliable systematics or theoretical predictions are used for data evaluation. The contents and principles of preparation of the ENSDF are described in detail in Refs. [1–3].

The most important data contained in the ENSDF are: for levels – excitation energy, spin, parity, time of life (or total width), decay branching ratio, electric and magnetic moment; for gamma-transitions – energy, intensity, multipolarity, mixing ratio; for alpha- and beta-decays – energy and intensity. These data are published regularly in *Nuclear Data Sheets* and (for $A < 45$) in *Nuclear Physics* compilations (for example, Ref. [4]).

The software for database operation with ENSDF exists and is being improved. This has obvious advantages: fast search, the preparation of data files for future application in special software, the possibilities for network uses, etc. There are several directions of special ENSDF software development. The programs provide the output information from ENSDF in a form similar to that of the *Nuclear Data Sheets* developed at the National Nuclear Data Center (NNDC), Brookhaven National Laboratory, USA. The NNDC on-line retrieval system has been in operation since 1986. The special programs MEDLIST and RADLIST [1,2] for medical applications are well known. Plans for development of the *Electronic Table of Isotopes* for the personal computer have been announced [5]. The nuclear radioactive decay gamma-radiation characteristics database was developed [6] in Lund University and the Institute of Technology (Sweden). A data library [7] based on ENSDF is known to be used as the bank of initial data for nuclear reaction model calculations. In Ref. [8] we proposed a method for "fast development" of specialized programs for the ENSDF operation. More than 15 programs were developed which gave the possibility of using ENSDF for various fields of application, including both basic research such as investigation of photonuclear reactions [9], and applied research such as, for example, gamma-activation analysis [10]. Several of these programs, used for the analysis of a large number of data on spins, parities, and spectroscopic factors of nuclear levels from ENSDF, helped us to predict several previously unknown spin values and evaluate the one-particle structure parameters for several nuclei [11,12].

The cited list of works illustrates one general feature of them. Each of the programs mentioned above searches for only a given subset of information from the ENSDF data bank. Future needs for new kinds of information will need new program development. This software organization method is not suitable when new needs appear relatively frequently.

Recently, the situation has changed noticeably. The availability of personal computers (PC), the development of database management systems (DBMS) with advanced interfaces, and convenient and powerful request languages

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allow the creation of a universal database (DB) using ENSDF. Essentially, the problem is to reorder the ENSDF data in such a manner that all possible requests for a subset of ENSDF are completely covered by the standard resources of DBMS.

This problem is naturally divided into several questions which have not been studied before. Is it possible to reorder the initial ENSDF treelike structure to a new structure which is suitable for using under DBMS on a PC? What part of the physically significant information would be lost after such a transformation? What is the efficiency of modern DBMS work with such large (about 100 Mb) data volumes? To what degree would the discussed system be amendable for future modifications and improvements?

Our first attempt at solving these problems and developing a database is described in the present work.

2. Brief ENSDF description

The structure of ENSDF is as follows [1,2]. A "data set" corresponding to one scheme (or table) of levels and transitions is the basic unit of structure of the file. Several data sets can exist for each nucleus. Each data set contains information on levels and radiations in this nucleus obtained from a single reaction or decay experiment for a given final nucleus. In addition, there are special data sets "Adopted Levels, Gammas" (one data set for one nucleus) in ENSDF which may be considered as the "best" or evaluated properties of the nuclear levels or radiations.

ENSDF is organized as a sequence of data sets for different nuclei and experiments, in ascending order by mass number A and charge Z.

The internal organization of a data set is the scheme of the levels followed by the transitions. Each data set consists of individual ordered records. The first – "I" record – identifies the whole data set and corresponds to the scheme (table) heading. Each of the following records consists of information on individual physical parameters; these parameters are elements of a general scheme of nuclear levels and transitions. "L" records contain ground and excited state characteristics; "G", "B", "E" and "A" records contain characteristics of the gamma-, beta-, electron capture and alpha transitions, respectively; "P" records contain parent nucleus properties (if the data set describes any decay); "Q" records contain energy characteristics of the nucleus; "N" records contain normalization coefficient values.

Each of these records has its own strict format. For example, the level energy is placed in columns 10 to 19 from the left in the "L" record, the energy uncertainty value is placed in columns 20 to 21, and so on for all values.

All records within any data set are ordered by nuclear levels and transition parameters similar to the individual physical parameters. For example, if gamma-transitions can deexcitate excited states, it means that "G" records are strictly connected with definite "L" records. The same situation holds for records for transitions populating definite levels – "A", "B", "E" records. At the same time, "N", "Q", "P" records are related directly to the whole data set.

Therefore, the different kinds of records form a hierarchical structure in ENSDF (Fig. 1). The first level of the hierarchy consists of "I" records, or data set headings. The next level consists of "N", "Q", "P" and "L" records; "G", "B", "E" and "A" records are also on this level if they describe transitions not placed in the scheme. The "G", "B", "E" and "A" records for transitions from or to definite nuclear states form the third level of the hierarchy.

It should be noted that this hierarchical structure of the ENSDF is realized by the ordering of the different kinds of records in the file. The fact that ENSDF has sequential organization plays an important role here. For instance, the "G" record must follow the "L" record for the level from which the gamma-transition occurs. Therefore, the positioning of any record in ENSDF carries quite important information. For this reason, one must solve the problem of the conservation of the hierarchical connections between different records when any ENSDF transformations are performed.

The information on some record types is omitted in this description: for example, text comments, continuation and reference decoding records. The reason is that these kinds of records are not included in the system described below at the present time; it is planned to include them in the next stage.

3. The database management system PARADOX

The database management system PARADOX (trade mark registered by Borland International) was chosen as the program tool for the new universal database on nuclear structure and decay. This choice was determined by two principal factors. First, this DBMS is known to be quite fast for large data volumes (at the present time, version 4.0 is declared to be the fastest in this class). Second, PARADOX has an advanced interface and a powerful query language, QBE (query by example).

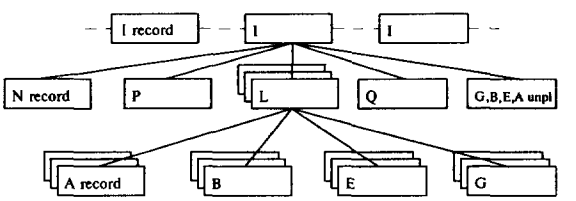

Fig. 1. The ENSDF records hierarchy.

Like the majority of DBMS with similar characteristics destined for the PC, PARADOX employs the relational data model, according to which "same-kind-data" are organized as "same-kind-tables". To construct a query in PARADOX, one enters on the screen representation of the corresponding table those values that are to be found. The operations +, −, *, /, <, >, = are appropriate for numerical fields, the context search for character fields, and the logical constructions for all types of fields. The constructed query can be saved as a file with any name, and a new query can be constructed from the previous one by means of an editor.

4. The creation of the relational database using the ENSDF information

To construct the universal relational database on nuclear structure and decay, one must combine the relational DBMS (in this case PARADOX) and ENSDF information. To do this one must transform the original file into a DBMS adaptable presentation. The preservation of the hierarchical relations in the original file is an important condition of this transformation. Since a table is the structural unit of any relational DB, and the ENSDF data set is an ensemble of ordered records of different kinds, the task of the construction of the necessary data tables on the basis of the existing data sets becomes the main problem.

To solve this problem, the whole original file ENSDF (the complete set of information for all nuclei) was decomposed into groups of records of the same kind, i.e. "I", "L", "G", "Q" records and others. Because they have the same format, such records being placed "each under the other" create the corresponding table automatically. The fragment of the "L" table obtained by extracting all "L" records is shown in Table 1. After this decomposition, the information from ENSDF appears as a set of tables "I", "L", "G", "Q", etc. It is clear that, without special actions, the information on the order of the records in the original file, which is responsible for hierarchical connections, may be lost.

To conserve this hierarchy, a special key system was developed. All records of each table were numbered. For each record the number assigned was declared as the "own" record key. In addition, "senior" keys were introduced for each record – one or several. The "senior" key of any record is the "own key value" of the hierarchically higher level corresponding to this record. For example, an "L" record has an own L-key. At the same time, this record has an I-key equal to the "own key value" (the number) of the "I" record identifying the data set which contains this "L" record (generally, all records of the same data set have the same I-key values). Any gamma-decays from this level (i.e. any "G" records corresponding to this "L" record) have assigned L-keys equal to the L-key of this "L" record (together with its own G-key). The record hierarchy recovered in this way is illustrated in Fig. 2.

5. The work of the universal relational nuclear structure and decay database

The ideas stated above were applied [13] at the Centre for Photonuclear Experiments Data of the Moscow State University Institute of Nuclear Physics (MSU INP CDFE) for the construction of the NESSY (New ENSDF Search SYstem) – the relational nuclear structure and decay database for IBM/PCs based on the ENSDF and the PARADOX combination. Special codes were developed for reorganizing the original file information, and for data import to the PARADOX system.

Table 1
Fragment of the "L" table, composed from "L" records of ENSDF

Mass	Symbol	Energy	$D(E)$	Spin and parity	Half-life	$D(H-l)$	Angular momentum transfer	Spect. str.	$D(S$ s)	Flag	Isom.	S?
50	Ti	6123	0		38 fs	+12 − 9						
50	Ti	6379	0		19 fs	LT						
50	Ti	6481	1		17 fs	LT						
50	Ti	6520	1		8 fs	+4 − 3						
50	Ti	6710	0		11 fs	4						
50	Ti	0		0+								
50	Ti	1554		2+	0.9 ps	3						
50	Ti	4311			2.5 fs	18						?
50	Ti	0		0+								
50	Ti	1550		2+	0.98 ps	9						
50	Ti	0										
50	Ti	1550		2+			2	0.68				
50	Ti	2670		4+			4	0.40				
50	Ti	3200					(6)			A		
50	Ti	3770										?

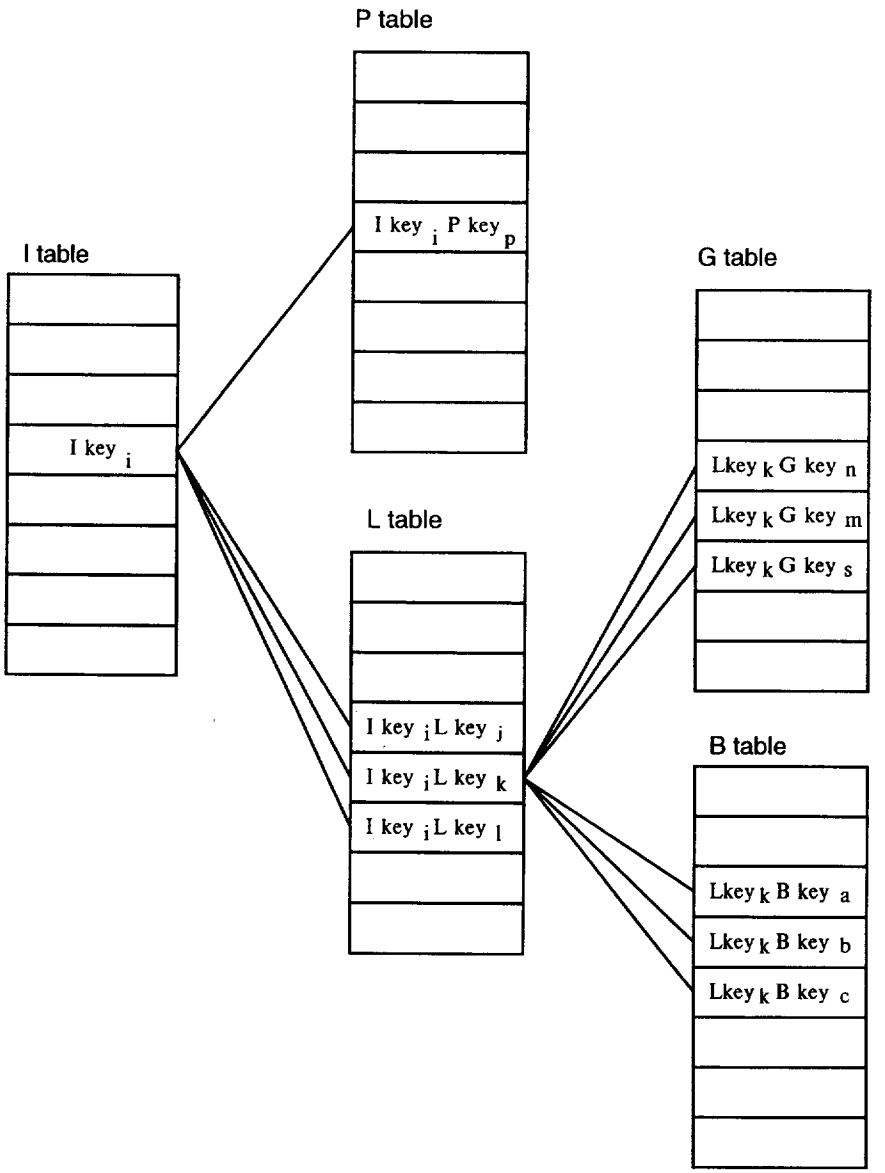

Fig. 2. Relations between the tables.

We have assumed that the ENSDF file is available; the composer of the ENSDF file is responsible for the quality of the information. Therefore, there are no additional verifications or changes of the data. The reliability of the import programs developed and the total NESSY system has been evaluated by means of a number of tests and by comparing their results with various well known data. There were no errors involved due to the NESSY development.

Therefore, the NESSY system is the result of merging two components: the standard PARADOX database management system, and the number of tables containing the ENSDF data. The compiled version of this system does not exist. The system uses PARADOX, version 3.5, and can be installed on any computer which can run this version. NESSY requires about 200 Mb of disk space. No additional requirements exist for a PC.

The data search in PARADOX may be carried out for the contents of any table field present in the system. This means that any physical parameter present in ENSDF can be the object of the search, and any demands can be specified for these parameters.

Similarly, any of the table fields for information retrieved may be obtained as a result of the search. Therefore, there is the possibility of retrieving any data from ENSDF corresponding to any query criteria.

Table 2
Fragment of the NESSY answer. See text for the query

Mass	Symbol	Energy	Spin and parity
36	Ar	10 319	2+
36	Ar	10 439	2+
36	Ar	10 558	2+
36	Ar	10 593	2+
36	Ar	10 613	1+, 2+, 3+
36	Ar	10 858	0+
36	Ar	11 027	3+
36	Ar	11 050	2+
36	Ar	11 222	1+, 2+, 3+
36	Ar	11 639	1+, 2+, 3+
39	Ar	11 312	1/2+
40	Ca	10 271	(3, 4, 5)+
40	Ca	10 321	1+
40	Ca	10 544	2+
40	Ca	11 418	4+
40	Ca	11 974	0+

Query for a single table. The simplest kind of query is one for a single table, because in this case both query demands and retrieved values correspond to the same physical parameters, i.e. levels, gamma-rays, etc.

For example, for the query "Nuclear levels", the following parameters may be requested:

- positive parity;
- excitation energy more than 10 MeV;

for which the following output information will be given:

- the nucleus (*Z*,*A*) which has such levels;
- excitation energy values of each of such levels;
- spin and parity values of each of such levels.

The result is presented in Table 2. The operating time for this query is about 40 s on a Philips P3370 (IBM/PC 386, 33 MHz).

Query for several tables. The key system described above is used to specify the query of information from several tables; in this case, the equivalences for the corresponding keys are stated. For example, for any characteristics of the parent states (P table) as an entry, we can obtain the characteristics of levels and gamma-rays observed in decays of these states (L and G tables), or decay modes (I table). Table 3 contains a full NESSY retrieval for this kind of query. The operating times of such queries are from several seconds to several dozen seconds. In particular, the possibilities of this system allow the restoration of the full level and transition schemes for any nucleus and data set, i.e. restore the initial original ENSDF structure for an individual data set (Table 4). This means that the adopted system of storing the keys preserves all the connections between the individual ENSDF records, and hence, all the information contained in the ordering of the ENSDF records is preserved.

The main features of NESSY compared with NUDAT, which is available on the BNL on-line service [1], are as follows.

(1) Configuration of both search conditions and output information, i.e. the set of physical quantities in NESSY is not limited. The queries are user defined by means of a combination of any fields from any tables. The NUDAT system consists of several menu items, which are searched according to a configuration ordered in advance. Particularly, with NESSY, the automatic formation of tables containing the search parameters and included in the common query configuration is possible, that is the fields of NESSY output tables can be used as the next search input data without additional input. This is especially suitable when a large number of searches is performed.

(2) The PARADOX query language allows requests to be posed by means of both values and the relations between them. A part of the output to a query for levels with energies differing by no more than 1 keV is presented in Table 5.

(3) The query language has several additional capabilities, such as the possibility of a search by the presence or absence of specified symbols in any table field, and the

Table 3
The NESSY answer to the query: decays of nuclei, masses $A < 45$, half-life times – hours or days

Mass	Symbol	Data set	Half-life	$D(H-l)$
7	Li	^{7}Be EC decay	53.29 d	7
24	Mg	^{24}Na β^- decay (15.020 h)	15.020 h	7
28	Al	^{28}Mg β^- decay	20.91 h	3
32	S	^{32}P β^- decay	14.26 d	4
33	S	^{33}P β^- decay	25.34 d	12
35	Cl	^{35}S β^- decay	87.51 d	12
37	Cl	^{37}Ar EC decay	35.04 d	4
38	Cl	^{38}S β^- decay	2.84 h	1
41	K	^{41}Ar β^- decay	1.827 h	7
42	Ca	^{42}K β^- decay	12.360 h	3
43	Ca	^{43}K β^- decay	22.3 h	1
43	Ca	^{43}Sc EC decay	3.891 h	12
44	Ca	^{44}Sc EC decay (2.442 d)	2.442 d	4
44	Ca	^{44}Sc EC decay (3.927 h)	3.927 h	8

Table 4
Levels and gamma-rays of ^{44}Sc from adopted levels, gammas (fragment)

Energy	$D(E)$	Spin and parity	Half-life	Isom.	S?	Energy-γ	$D(E)$-γ	Relative intensity	$D(R$ i)	Multipolarity	Mix ratio	Coin p	Coin f	Energy − Energy-γ
829.00	2.00				?	479.20								349.80
						829.00								0.00
763.10	0.40	3+	0.22 ps			528.40		7.5	22E − 1					234.70
						763.10		100.0	22E − 1	$M1(+E2)$	+0.06			0.00
666.70	0.40	1+	49 fs			666.70		100.0		$M1(+E2)$	+0.09			0.00
630.94	0.13	4−	0.40 ns			206.17		18.8	21E − 1					424.77
						281.10		100	5	$E1(+M2)$	+0.02			349.84
						396.24		90	5	$E2(+M3)$	−0.02			234.70
531.50	0.20	3	35 ns			181.66		4.1	21E − 1					349.84
						296.80		100	4	$D(+Q)$	+0.02			234.70
						463.65		20	4	$Q(+O)$	−0.02			67.85
						531.50		80	4	$D(+Q)$	+0.04			0.00
424.77	0.08	3−	0.38 ns			190.07		45	4	$M1(+E2)$	−0.02			234.70
						356.92		100	4	$E2(+M3)$	0.00			67.85
						424.77		28	4	$E1(+M2)$	−0.03			0.00
349.84	0.09	4+	3.1 ns			349.84		100.0		$E2(+M3)$	+0.01			0.00
271.13	0.11	6+	2.442 d	M		271.24	10E − 3	100.0		$(E4)$				−0.11
234.70	0.20	2−	6.1 ns			88.45		2.9						146.25
						166.85		45	3	$M1(+E2)$	−0.02			67.85
						234.70		100	3	$E1(+M2)$	0.00			0.00
146.25	0.05	0−	49 μs			78.38	4E − 2	100.00	3E − 2	$(M1)$				67.87
						146.23	6E − 2	0.10	3E − 2					0.02
67.85	0.04	1−	153 ns			67.85	4E − 2	100.0		$E1(+M2)$	0.01			0.00
0.00		2+	3.927 h											

possibility of performing arithmetic and other operations over searched values. In the example given above, an additional condition was added: the existence of any information about the half-life of the level, i.e. the existence of a non-empty record in "half-life time" in the "L"-table.

NESSY allows one to solve the tasks for which specialized systems were developed earlier in a simple manner. So, for example, "The ENSDF Radioactivity Data Base" [6] mentioned above allows the solution of the following tasks: (i) retrieving the radioactive decay gamma-lines with energies closest to the requested ones; (ii) retrieving a full listing of the gamma-lines observed for the decay requested. It is clear that NESSY allows these possibilities by combining two ordinary query tasks for G and I tables by connecting them by means of the I-key (see Table 6).

The powerful capabilities of NESSY are illustrated by examples of its application in the MSU INP CDFE to the solving of two data search tasks related to concrete nuclear physics problems.

Nuclear ecology. It was necessary to follow the decay chains of every radioactive isotope requested (about 250

Table 5
Fragment of the NESSY answer: pairs of levels with coinciding energies

Mass	Symbol	Energy	$D(E)$	Half-life	Mass-1	Symbol-1	Energy-1	$D(E)$-1	Half-life-1
100	Mo	535.60	0.30	12.2 ps	100	Mo	535.60	0.30	12.2 ps
100	Mo	535.60	0.30	12.2 ps	130	Xe	536.09		6.4 ps
100	Mo	535.60	0.30	12.2 ps	133	La	535.60	0.02	62 ns
100	Mo	535.60	0.30	12.2 ps	172	Tm	535.14	0.00	1.22 ns
100	Mo	535.60	0.30	12.2 ps	81	Br	536.22	0.11	34.6 μs
100	Mo	694.40	0.60	1.7 ns	100	Mo	694.40	0.60	1.7 ns
100	Mo	694.40	0.60	1.7 ns	148	Ho	694.40		2.35 ms
100	Mo	694.40	0.60	1.7 ns	96	Nb	694.46	0.22	1.4 ns
100	Ru	539.59	0.05	10.8 ps	100	Ru	539.59	0.05	10.8 ps
100	Ru	539.59	0.05	10.8 ps	151	Pm	540.37	0.01	0.1 ns
100	Ru	539.59	0.05	10.8 ps	172	Yb	540.00	0.02	17.2 ps
100	Ru	539.59	0.05	10.8 ps	191	Au	540.30	0.80	10 ns
100	Ru	539.59	0.05	10.8 ps	191	Ir	538.86	0.02	10.2 ps
100	Ru	539.59	0.05	10.8 ps	84	Zr	540.00	0.50	14.1 ps

Table 6
Gamma-rays with energies closest to 1000 keV (within 30 keV interval) from the decays of nuclei with $A < 40$

Mass	Symbol	Data set	Energy	$D(E)$
8	Li	^{8}He β^- decay	981	
10	B	^{10}C EC decay	1022	14E − 2
15	N	^{15}C β^- decay	1012	
16	O	^{16}N β^- decay	988	4E − 1
23	Ne	^{23}F β^- decay	1017	2E − 1
24	Mg	^{24}Al β^+ decay (2.066 s)	998	4E − 1
24	Mg	^{24}Na β^- decay (15.020 h)	998	4E − 1
25	Mg	^{25}Al β^+ decay	975	10E − 2
25	Mg	^{25}Na β^- decay	975	7E − 2
25	Mg	^{25}Na β^- decay	990	2E − 1
25	Na	^{25}Ne β^- decay	980	2E − 1
26	Mg	^{26}Na β^- decay	1002	3E − 1
27	Al	^{27}Mg β^- decay	1014	4E − 2
27	Al	^{27}Si EC decay	1014	4E − 2
27	Mg	^{27}Na β^- decay	985	2E − 1
28	Al	^{28}Mg β^- decay	983	5E − 1
28	Al	^{28}Mg β^- decay	1014	5E − 1
39	Ar	^{39}Cl β^- decay	986	14E − 2

nuclides) and indicate decay mode, final nucleus, half-life, and branching ratio values for every decay. Since the final nucleus of the majority of decays is the parent nucleus for the next decay, the "query chain" scheme was achieved. The appearance of any stable isotope as a final one is an end-point for every query chain. The "query chain" scheme is presented in Fig. 3. The resulting table for the case described contained information on about 500 elementary decays.

Atomic power station waste utilization. For the mathematical modelling in this field, the data on specific nuclei was required and the following parameters were specified:

- indicate all levels with known gamma-decays and renormalize the data obtained so that the sum of intensities for every level is equal to 1;
- find and indicate all metastable states;
- determine if radioactive decays of the nucleus exist (both for ground and excited states) and, if so, indicate their modes, half-life times, and the average excitation energy of the final nuclei;
- give a complete listing of such states.

To solve this task, a sequence of elementary queries for NESSY was developed, and the information requested was obtained for a large number of nuclides.

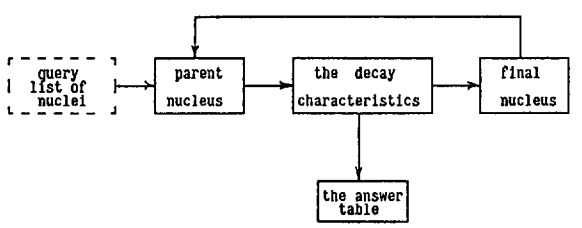

Fig. 3. The NESSY query system for obtaining nuclear decay full chains.

In general, the first experience with using NESSY testifies that it is a very powerful and convenient tool for both fundamental and applied research in a wide range of fields of science and technology.

References

[1] T.W. Burrows, Nucl. Instr. and Meth. A 286 (1990) 595.
[2] J.K. Tuli, National Nuclear Data Center, Brookhaven National Laboratory, Report BNL-NCS-51655-Rev. 87, 1987.
[3] M.R. Bhat, Brookhaven National Laboratory, Report BNL-45306, 1989.
[4] F. Ajzenberg-Selove, Nucl. Phys. A 433 (1985) 1.
[5] J.Z. James, Books of Abstracts of 4th Annu. Scientific and Technical Conf. of the Nuclear Society, Nuclear Energy and Human Safety, NE-93 (June 28–July 2), 1993, p. 96.
[6] L.P. Ekstrom and L. Spanier, KDK-110, NEANDC(OR)-162/U, INDC(SWD)-23/L, Stockholm, 1990, p. 16.
[7] O. Bersilon and J. Blachot, Service de Physique Neutronique et Nucleaire, Centre d'Etudes de Bruyeres-le-Chatel, Report NEANDC(E) 246/L, INDC(FR) 071/L, 1991.
[8] I.N. Boboshin and V.V. Varlamov, Voprosy Atomnoj Nauki i Tekhniki, Seriya: Yadernye Konstanty, 3 (1985) 42; I.N. Boboshin and V.V. Varlamov, Report IAEA, INDC(CCP)-297/GE, 1985.
[9] B.S. Ishkhanov, I.M. Kapitonov and I.A. Tutyn', Phys. At. Nucl. 56(8) (1993) 991.
[10] M.G. Davydov, V.V. Kishel'gof, B.A. Chapyzhnikov and V.A. Shcherbachenko, At. Energ. [Sov. J. At. Energy] 62 (1987) 33.
[11] I.N. Boboshin, V.V. Varlamov, B.S. Ishkhanov and I.M. Kapitonov, Nucl. Phys. A 496 (1989) 93.
[12] I.N. Boboshin, V.V. Varlamov and E.V. Nartova, Izv. Rossijskoj Akad. Nauk, Ser. Fiz. 56 (1992) 93.
[13] I.N. Boboshin, V.V. Varlamov and S.K. Trukhanov, Int. Conf. on Nucl. Data for Science and Technology, Book of Abstracts, ORNL, USA, 1994, p. B29.