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Technical note

Nuclear reaction and structure data services of the National Nuclear Data Center

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Abstract

The mission of the National Nuclear Data Center (NNDC) includes collection, evaluation, and dissemination of nuclear physics data for basic nuclear research and applied nuclear technologies. In 2004, to answer the needs of nuclear data users, NNDC completed a project to modernize storage and management of its databases and began offering new nuclear data Web services. The principles of database and Web application development used at NNDC are described. Examples of nuclear structure, nuclear reaction and bibliographical database applications along with a number of nuclear science tools and codes are presented.

1. Introduction

Nuclear data activities started at Brookhaven National Laboratory (BNL) in 1951 in a group that would become the National Nuclear Data Center (NNDC) in 1977 (Pearlstein, 1970). The center's objective is to collect, evaluate, and disseminate nuclear physics data for basic nuclear research and applied nuclear technologies. The NNDC maintains and contributes to the nuclear structure (ENSDF, XUNDL, NSR) and reaction (ENDF, CSISRS, CINDA) databases[1] as well as several databases derived from these primary databases. The center prepares photo-ready copy for Nuclear Data Sheets journal, publishes Nuclear Wallet Cards booklets and neutron cross sections reference books formerly known as BNL-325 (Mughabghab, 2006; Mughabghab et al., 1981, 1984; McLane et al., 1988) and provides coordination and maintains databases for the Cross Section Evaluation Working Group (CSEWG), and United States Nuclear Data Program (USNDP).

The NNDC has been providing remote electronic access to its databases and other information since 1986. Access was originally by modem and via HEPNET, the US Department of Energy-sponsored High Energy Physics Network which employed the DECNET protocol, and later the TCP/IP protocol. Remote login via Telnet was used on HEPNET and the INTERNET. This electronic service was hosted on DEC computers using the VMS operating system and Oracle 6.0 CODASYL DBMS database software. Implementation of the World Wide Web protocol started in 1994. The Web service was based on the Ohio State University Web server.

This system has proven to be robust and scalable, providing excellent customer service for more than 18 years. However, there have been dramatic information technology developments over the last 15 years. The Open VMS operating system and CODASYL DBMS database software did not keep pace with these technological advances. It became increasingly difficult to support the NNDC Web

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[1] A complete description of nuclear data, software industry terms and acronyms, is presented in Appendix 1.

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site, satisfy all cyber security requirements, redundancy, international compatibility, and the future growth requirements with the existing system. The current industry standards are largely based on UNIX operating system, Relational Database Management System (RDBMS) software, Structured Query Language (SQL), and Java programming language.

In order to improve the quality of nuclear data services and take advantage of latest software and hardware developments, the NNDC started to work on a migration project in 1999, following a basic assessment of future options. This exploratory work culminated at an International Workshop on Relational Database and Java Technologies for Nuclear Data, held at BNL, September 11–15, 2000.

As a result of the workshop, the NNDC in partnership with the IAEA's Nuclear Data Section (Humbert et al., 2004) embarked on a project to migrate its databases to a UNIX-based relational database environment and significantly upgrade Web Services employing the latest technologies (Pronyaev et al., 2002). The migration project was successfully completed and the new NNDC nuclear data Web service made available to the public in April 2004. During 2004, users from more than 11,500 organizations visited NNDC's Web site and made 5.6×10^5 database retrievals, a 66% increase compared to year 2003.

In the following sections, we present current status and results of the database migration project, which creates a foundation for the next generation of nuclear data Web services. First, we describe hardware and software computer environments, followed by software application developments and careful analysis of Web implementations.

2. New NNDC computer environment

The new NNDC computer environment is based on DELL/Linux platforms which includes Sybase relational database software and extensive use of Java technologies (Sybase, Inc.; Rankins et al. (1996); Bergsten (2002)).

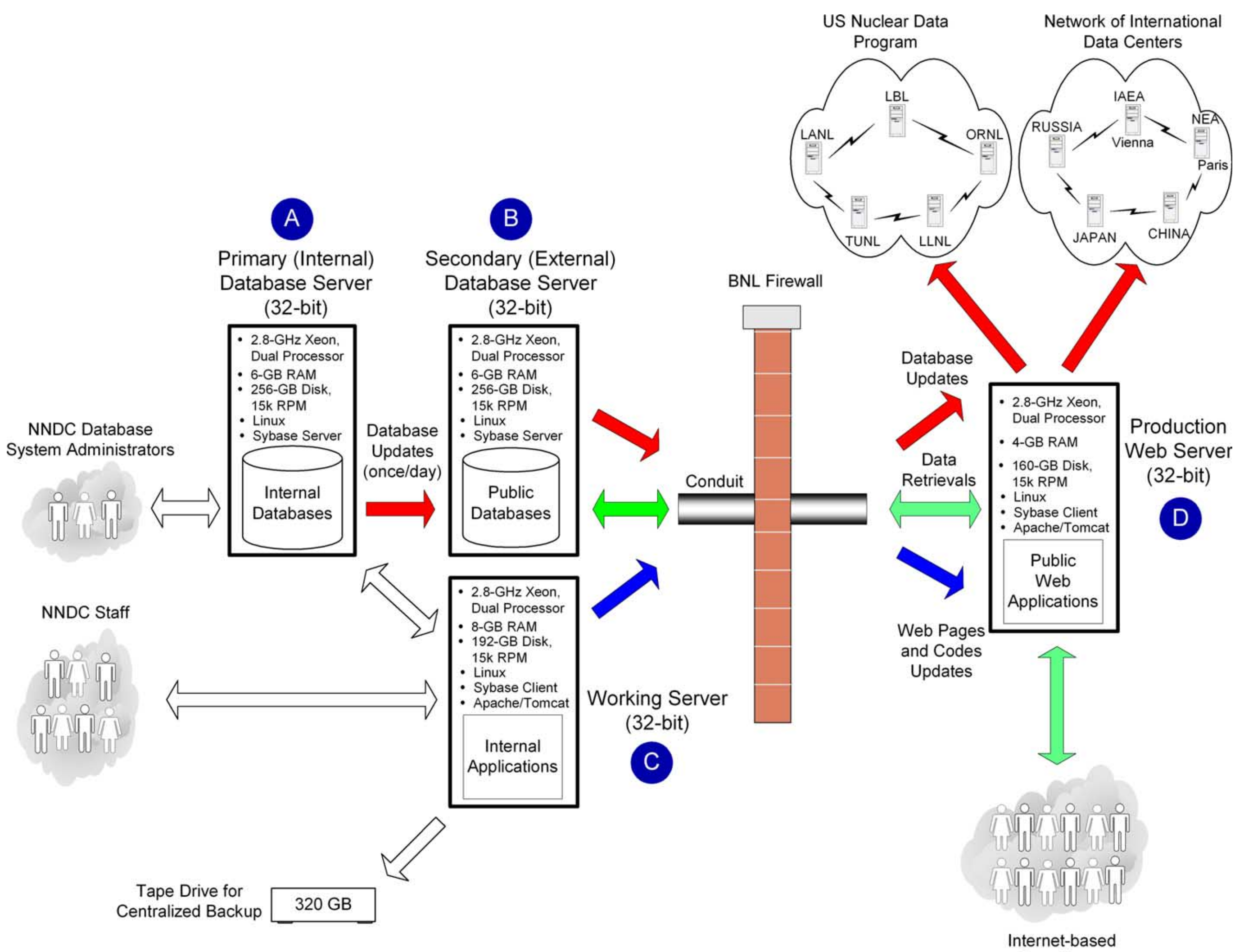

Fig. 1. Schematic view of the NNDC database computer system. New nuclear data content is propagated from primary (A) to secondary (B) database server which is connected to the Web server (D). Working server (C) is mostly used as Java testing and development environment.

2.1. NNDC computer hardware and software

To provide more robust, scalable architecture, satisfy cyber security requirements and protect nuclear data services from a single-point failure, the Web server and two database servers (primary and secondary) are physically separated. The Web server is connected to the secondary database server while the primary database server is used for updates which are later propagated to the secondary server. All Java and Web site testing and development are performed on a working server that closely replicates the software environment installed on the Web server. The schematic view of the new system is presented in Fig. 1.

The new system consists of two database servers (DELL PowerEdge 6600, 2 × 2.8 GHz Intel Xeon processors, 6 GB RAM, 15 kRPM hard drive), a Web server (DELL PowerEdge 2650, 2 × 2.8 GHz Intel Xeon processors, 4 GB RAM), and a working server (DELL PowerEdge 4600, 2 × 2.8 GHz Intel Xeon processors, 8 GB RAM). The database servers are running Sybase ASE 12.5 RDBMS software, while the Web server has the Apache 2/Tomcat 5/mod_jk 1.2.10 (The Apache Software Foundation; The Apache Jakarta project) Web production environment installed. All servers are running the Red Hat Linux operating system.

2.2. NNDC database and web software application development

The NNDC databases were migrated using the hardware and software described above. Typically each database migration task was composed of the following five components

- Schema design.
- Data loading, update and general maintenance program development.
- Data preparation and quality control program development.
- Web-based retrieval development.
- Transfer of production activities to Linux/Sybase environment.

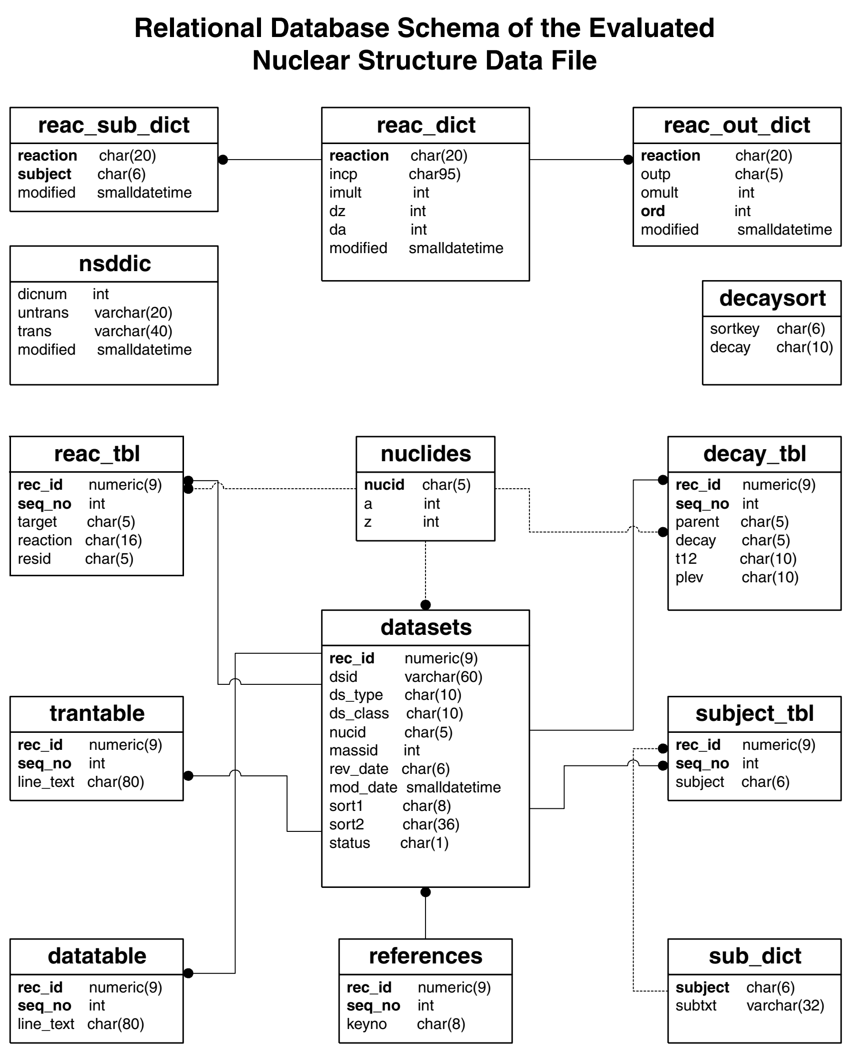

Fig. 2. Example of relational database schema. The evaluated nuclear structure data file (ENSDF) database schema consists of 14 tables and 12 relationships which enforce referential integrity between tables.

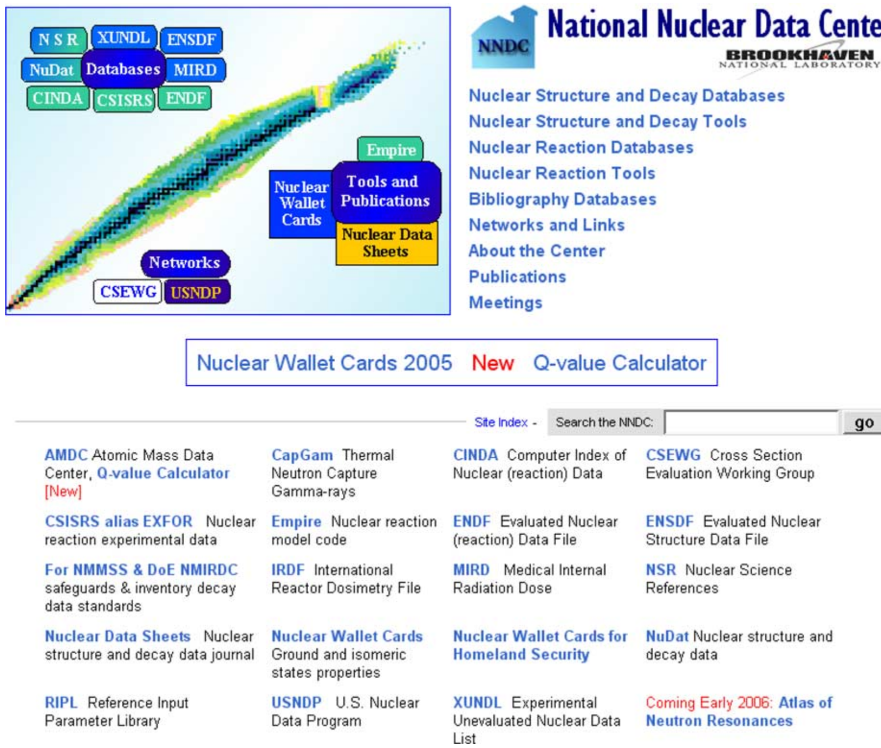

Fig. 3. Front page of the NNDC Web Services: Nuclear Data Portal (www.nndc.bnl.gov). All elements of the page, including graphic images, are hyperlinked.

The database schema[2] design and development were determined by the particular database requirements; each database consists of tables, indexes, and relationships with enforced referential integrity. As an example, the ENSDF database schema (Tuli, 1996, 2001; Winchell, 2005) are shown in Fig. 2. The Evaluated Nuclear Structure Data File is made up of a collection of "data sets" that are organized by their mass number and contain the following information: mass chain summary, references used in all data sets for a given mass number, adopted levels and γ-ray properties for each nuclide, evaluated results of a single type of experiment and combined evaluated results of a number of experiments (Tuli, 2001). Data set structure is reflected in the central and lower part of the ENSDF database schema and database dictionaries are shown in the upper part of the schema. In designing the new database structures, it was important to maintain all previous functionality, and to be able to retrieve data in the legacy ASCII text "exchange" format.

A combination of Java codes with embedded SQL statements is used for database loads, updates, maintenance, data preparation, and quality control tasks. Most of the Web applications were completely re-written using Java Server Pages (JSP), Java Servlets, and Javascript technologies to provide up-to-date, user-friendly Web interfaces for nuclear data users. JSP Web technologies are based on JavaBeans specification for Java classes, which provides Web applications with data access and retrieval methods (Bergsten, 2002). In addition to new codes, many legacy Fortran codes were modified to access the new databases.

The new hardware/software system went into operation and has demonstrated high performance and reliability with a down time of less than 1%.

3. Nuclear data portal

New Web interfaces integrated with relational databases created a Nuclear Data Portal (www.nndc.bnl.gov) launched on April 19, 2004 (Pritychenko et al., 2004,). The portal is a Web-based interface which gives users access to all Web and database applications through a single screen on their computer. The Nuclear Data Portal contains nuclear structure, decay and reaction data, as well as bibliographical information. Its major features include: new hardware architecture based on robust and scalable DELL servers running Linux and relational database software (Sybase), Java solutions for Web applications, easy to navigate, active Graphic User Interfaces (GUI) and a Google search engine.

The new Web-based nuclear data retrieval system or Nuclear Data Portal is tightly integrated with nuclear reaction (CSEWG) and structure (USNDP) evaluations and compilation efforts. The portal is shown in Fig. 3. The new Nuclear Data Portal has resulted in a significant

[2] The overall description of the database logical structures that is defined by the data definition language (Lorents and Morgan, 1998).

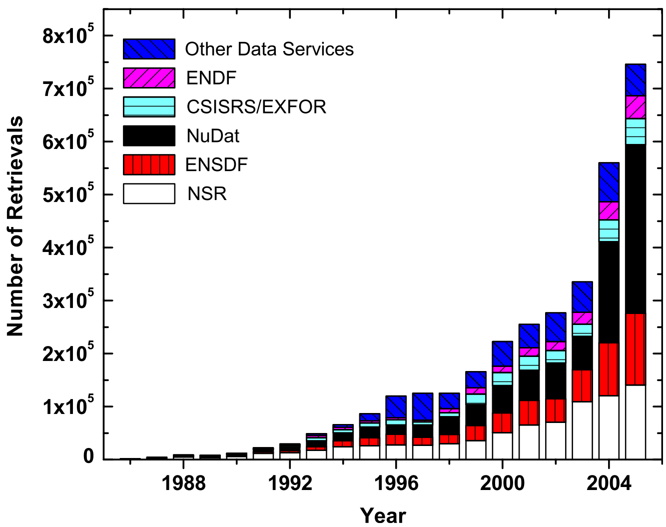

Fig. 4. Electronic nuclear data retrievals from the NNDC over the last 20 years. Data retrievals for 2005 are estimated.

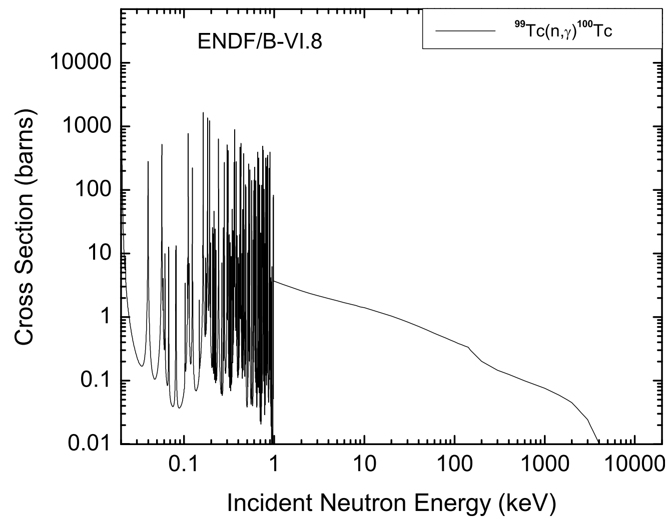

Fig. 5. ENDF/B-VI.8 evaluated neutron-capture cross section from 0.02 keV to 20 MeV is shown for important waste transmutation nucleus ^{99}Tc.

increase in the NNDC Web data retrievals compared with the previous service. Fig. 4 summarizes results for Web data retrievals. Results for five major databases indicate that data retrievals for calendar year 2004 vs. 2003 increased for CSISRS/EXFOR by 74.5%, ENDF by 53.5%, ENSDF by 65.5%, NSR by 10.2% and NuDat by 205.3%. The relatively small increase for NSR database reflects the fact that a Java version of NSR was available in 2003 with a 15% annual growth. If this trend continues, there will be about 7.5×10^5 retrievals in 2005. NNDC statistics include the data retrievals only and do not count any Web page access that does not result in information being retrieved. For more explanation about the statistics (see Burrows, 2003; Turner, 2004).

4. Nuclear reaction data services

Nuclear reaction data services were substantially improved to provide a better access to reaction data evaluations and compilations (Zerkin et al., 2005). New Web interfaces for the Evaluated Nuclear Data File (ENDF), the nuclear reaction experimental data (CSISRS/EXFOR), and the Computer Index of Nuclear (reaction) DAta (CINDA) databases, developed in collaborative effort with the IAEA's Nuclear Data Section (Humbert et al., 2004), provide a wide range of options for data retrievals and analysis using standard and interpreted text formats as well as graphic tools. New nuclear reaction services distinguish themselves via the simple manner of creating on-line database queries and the extensive use of graphics. A brief description of the reaction databases is presented below.

4.1. Evaluated nuclear (reaction) data file (ENDF)

The ENDF reaction database contains recommended data from the United States ENDF/B-VI.8 library McLane (1996) as well as from the other international evaluated nuclear reaction libraries: BROND, CENDL, JEFF, and JENDL (Blokhin et al., 1994; Chinese Nuclear Data Center, 1991; Jacqmin et al., 2002; Shibata et al., 2002). The data are stored in the ENDF-6 format and include most nuclides of practical relevance (329 in total for ENDF/B-VI) for neutron-induced reactions up to 20 MeV. Some evaluations extend up to 150 MeV. This data serves as the principal input for neutronics calculations, including nuclear reactor design and operation, national security, criticality safety, accelerator design, radiation protection, radiotherapy, and detector simulation.

ENDF database output is available in graphic and text formats. ENDF/B-VI.8 output for evaluated cross section of important in waste transmutation reaction ^{99}Tc $(n,\gamma)^{100}$Tc is shown in Fig. 5. The current version of the ENDF library is ENDF/B-VI.8; the ENDF/B-VII library is scheduled for release by the middle of 2006.

4.2. Experimental nuclear reaction data (CSISRS alias EXFOR)

The CSISRS (Cross Section Information Storage & Retrieval System), alias EXFOR (EXchange FORmat) data library contains experimental nuclear reaction data for incident neutrons, charged particles, and photons. It includes more than 15,500 experiments and covers nearly all of neutron-induced reaction experimental data up to the pion threshold. The library is less complete for charged particle induced reactions (in general $A \leqslant 12$) and photon experiments. In the recent years, the number of charged particles compilations is rising faster than others. The EXFOR compilations are coordinated by the Nuclear Reaction Data Centers Network (NRDC) (Nichols, 2005).

5. Nuclear structure data services

Nuclear structure data services were significantly upgraded to improve capabilities and user friendliness for the Evaluated Nuclear Structure Data File (ENSDF), Nuclear structure and decay Data (NuDat), eXperimental Unevaluated Nuclear Data List (XUNDL) and Medical Internal Radiation Dose (MIRD) databases (Tuli, 2001; Sonzogni, 2005; McMaster University Data Evaluation; Medical Internal Radiation Dose; Burrows, 1990). The new ENSDF Web services significantly improve and simplify ENSDF datasets retrievals, while a new NuDat 2.1 Web service enhances search and presentation capabilities for nuclear data, and provides a more convenient way to search for specific levels and γ-ray energies.

5.1. Evaluated nuclear structure data file (ENSDF)

The ENSDF evaluated nuclear structure and decay database contains recommended data for all evaluated nuclides, currently 2929, organized in over 15,452 individual datasets (Winchell, 2005). It serves as a principal source of data for nuclear structure research, nuclear spectroscopy applications, the databases MIRD and NuDat, and publications such as Table of Isotopes (Firestone et al., 1996). Nuclear structure information in the ENSDF database is organized by dataset. Each dataset contains evaluated nuclear structure information from reaction or decay and conforms to the internationally adopted ENSDF format (Tuli, 1996, 2001), which permits further processing by a large number of existing programs. Contributions to ENSDF come from evaluators of the international network of Nuclear Structure and Decay Data (NSDD) (Tuli, 1996; Nichols, 2005) while the database is maintained by NNDC.

5.2. Nuclear structure and decay data (NuDat)

NuDat contains evaluated (recommended) nuclear structure and decay data for 2932 nuclides, with about 1.40×10^5 levels, 2.04×10^5 γ-ray energies, etc. (Sonzogni, 2005). It is a derived database, information is extracted from ENSDF and Nuclear Wallet Cards. The NuDat software application was completely redesigned and uses the latest Java graphic technologies. Currently it is the most popular application on Nuclear Data Portal (Web Watch, 2004). The new NuDat 2.1 software supports searches on parameters such as nuclide or parent, energy levels, decay modes, J^π, $T_{1/2}$ and E_γ.

The NuDat 2.1 main page includes an interactive chart of nuclei. A cell in a chart represents a known nuclide with the number of neutrons on the horizontal axis and the number of protons on the vertical axis. The color of the cell indicates the ground state half-life or predominant decay mode. NuDat 2.1 interactive chart of nuclei is shown in Fig. 6. NuDat outputs include a complete list of levels and level schemes. The level scheme for selected levels in neutron-rich nucleus of ^{178}Hf (Schwarzschild, 2004) is shown in Fig. 7. This case is important because of ongoing research on energy storage in nuclear isomers.

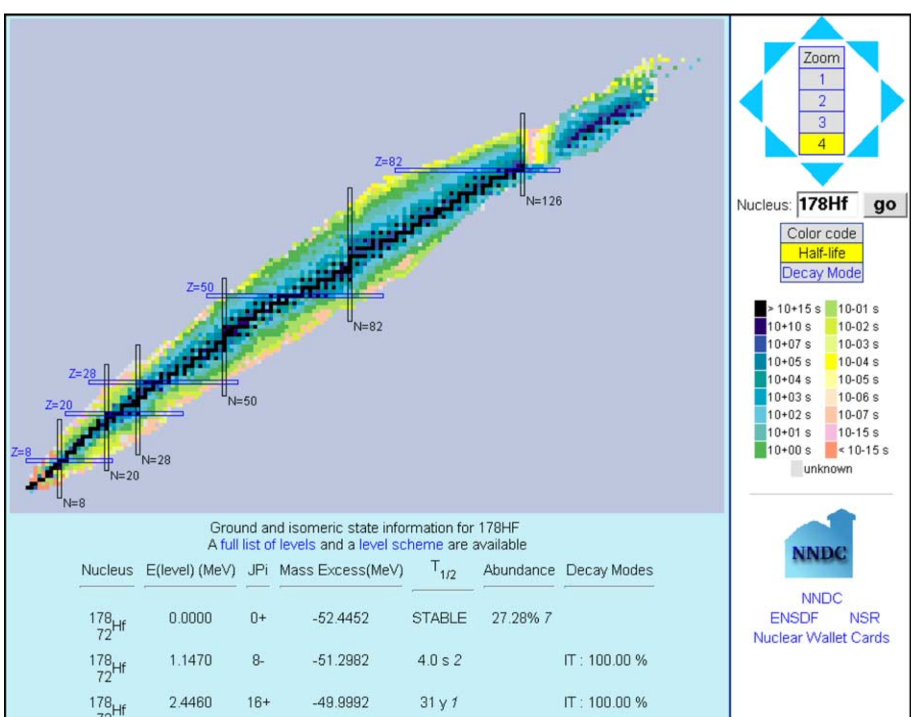

Fig. 6. NuDat 2.1 (www.nndc.bnl.gov/nudat2) data retrieval for ^{178}Hf displays ground and isomeric state information, see bottom of the figure. A full list of levels and level scheme are also available.

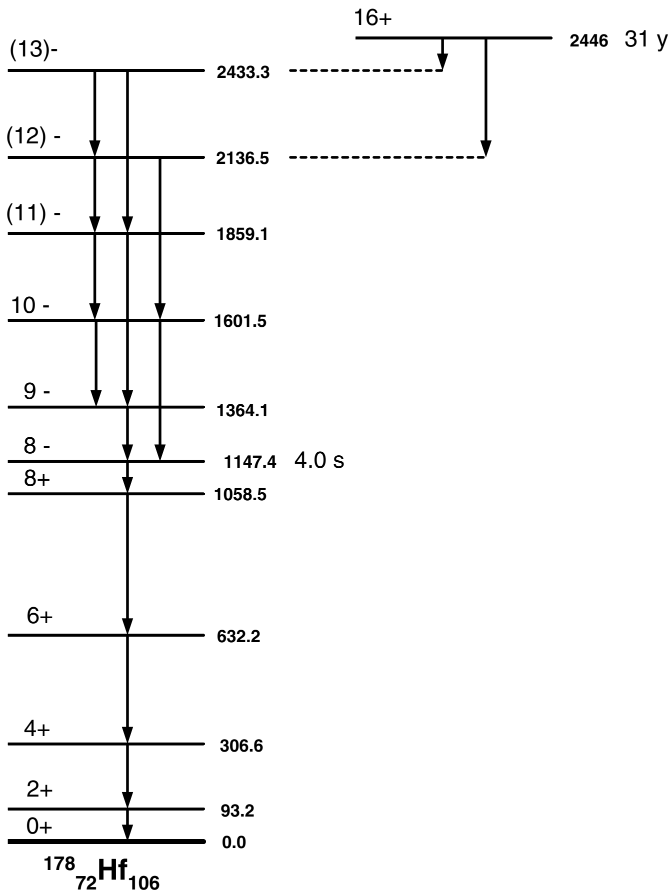

Fig. 7. NuDat 2.1 level scheme of ^{178}Hf displays 16^+ and $T_{1/2} = 31$ y isomer of ^{178m2}Hf. The isotope decays to $(13)^-$ and $(12)^-$ states of ^{178}Hf.

6. Nuclear bibliography data services

Bibliography data services such as Nuclear Science References (NSR) and Computer Index of Nuclear (reaction) DAta (CINDA) databases (Winchell, 2005; Computer Index of Nuclear (reaction) Data, 2002) are described below.

6.1. Nuclear science references (NSR)

NSR is an indexed bibliography of nuclear physics papers and reports containing over 1.8×10^5 nuclear science references, indexed according to content (Winchell, 2005). The contents span almost 100 years of research, and currently covers 80 journals with about 4200 new articles added per year. The database is updated by NNDC on a weekly basis to stay current with published literature.

In addition to standard reference, author, and title information, most entries in the NSR database include "keyword abstracts" to allow a search for references relevant to specific quantities or topics. Where available, digital object identifier (doi) links to publisher's pages are provided. Quick retrievals by author or nuclide, as well as indexed or text searches, and keynumber retrievals, are available. Search parameters for indexed retrievals include nuclide, author, subject, reaction, target, incident or outgoing particle, and topic. These parameters can be combined to create on-line queries and produce more focused results. It also contains links to ENSDF and XUNDL databases, where relevant.

6.2. Computer index of nuclear (reaction) data (CINDA)

The CINDA database contains neutron-induced reaction bibliographic information, including experimental, theoretical, and evaluated references (Computer Index of Nuclear (reaction) Data, 2002). It contains references to 2.75×10^5 reactions from 5.5×10^4 works primarily compiled by members of the NRDC (Nichols, 2005).

7. Tools and publications

NNDC provides access to many other resources of interest to the nuclear scientific community. These include calculational tools, computer codes, data libraries, and publications. Nuclear physics tools and publications, such as Empire (see next paragraph), Nuclear Wallet Cards, Nuclear Data Sheets and Q-value Calculator (QCalc) were upgraded and integrated into the Nuclear Data Portal.

7.1. Empire

Empire is modular nuclear reaction code for advanced calculation of nuclear reactions using various theoretical models (Herman et al., 2002). It consists of a number of linked FORTRAN codes, input parameter libraries, and the experimental data library (CSISRS/EXFOR). Application of Empire-2.19 code for the ^{232}Th(n,f) neutron fission cross section calculation (Herman et al., 2005) is shown in Fig. 8.

7.2. Nuclear wallet cards

The Nuclear Wallet Cards publication, currently in its seventh edition (Tuli, 2005), contains up-to-date ground and isomeric states properties of all known nuclides. The

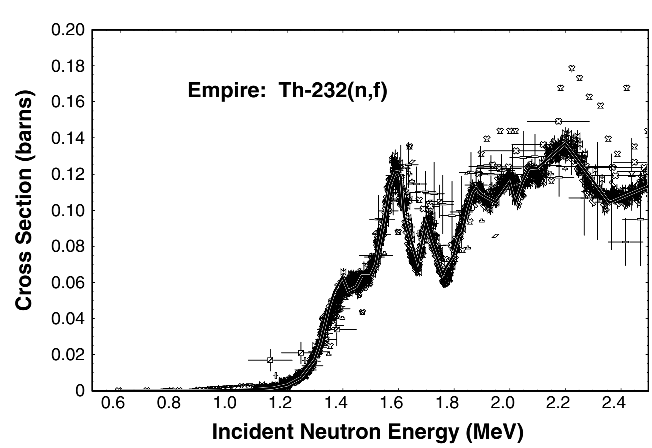

Fig. 8. ^{232}Th(n,f) neutron fission cross section calculated with the recent version of Empire 2.19. Experimental data are taken from 12 different references (Cross Section Information Storage & Retrieval System).

sixth edition of Nuclear Wallet Cards (Tuli, 2000) has been adopted by the US Department of Energy, Nuclear Materials and Safeguards System as their decay data standard.

A version tailored for Homeland Security needs is also available (Tuli, 2004). Nuclear Wallet Cards for Radioactive Nuclides include nuclear properties of $T_{1/2} \geqslant 1$ h nuclides and consists of two tables. The first one provides half-life, major radiations, and major γ-ray information for 737 nuclides. The second table contains information on 944 γ-rays and parent nuclides sorted by energy from 101 to 2951 keV.

In addition to Web versions, Nuclear Wallet Cards are distributed as booklets and as Palm Pilot applications.

7.3. Nuclear data sheets

NNDC edits and produces the *Nuclear Data Sheets* journal. The journal, published by Elsevier, is devoted to the publication of evaluated nuclear structure and decay data. These articles contain recommended values based on a careful evaluation and analysis of all available experimental results dealing with nuclear properties. An index to recent issues of the *Nuclear Data Sheets* is also available on the Web.

7.4. Q-value calculator

QCalc is a software application for the calculation of decay or reaction Q-values and threshold energies using the data from 2003 Atomic Mass Evaluation (Wapstra et al., 2003). The latest version of QCalc is written in Java.

8. Conclusion

The new Nuclear Data Portal of the National Nuclear Data Center (www.nndc.bnl.gov) is a result of the successful completion of the database migration project that was carried out by NNDC for the US Nuclear Data Program. The Nuclear Data Portal is based on a DELL/Linux solution with extensive use of Sybase relational database management software, SQL, and Java Web technologies.

The portal brings together nuclear structure, reaction and bibliography Web services, publications, and tools. It provides a unique access to many nuclear physics resources and creates a single site where nuclear data users can find tools and data to help solve science, industry and homeland security problems and challenges.

Use of electronic nuclear data services continues to grow in a near-exponential way. This is illustrated in Fig. 4, showing the growing number of downloads from the NNDC databases since 1986, a trend supported by similar experience of other nuclear data centers. It appears that the user demand is far below saturation as demonstrated by accelerated use of new services in 2004. We are confident that the portal has considerable potential to meet growing demands in the next years. On the other hand, the present paper demonstrates that nuclear databases, if utilized in a wise and innovative way, offer opportunities for far more proficient service in future.

Acknowledgements

We are grateful to D. Rochman and M. Blennau for a careful reading of the manuscript and useful discussions and suggestions. This work was funded by the Office of Nuclear Physics, Office of Science of the US Department of Energy, under Contract No. DE-AC02-98CH10886 with Brookhaven Science Associates, LLC.

Appendix 1

Nuclear data, software industry and information technology terms and acronyms are presented in the following table

Selected nuclear data, software industry and information technology terms and achronyms

Term or Acronym	Description	Reference
Apache	HTTP server	The Apache Software Foundation
BROND	Russian Evaluated Nuclear Data Library (reaction)	Blokhin et al. (1994)
CENDL	Chinese Evaluated Nuclear Data Library (reaction)	Chinese Nuclear Data Center (1991)
CINDA	Computer Index of Nuclear DAta (reaction)	Computer Index of Nuclear (reaction) Data (2002)
CSEWG	Cross Section Evaluation Working Group	Cross Section Evaluation Working Group (CSEWG)
CSISRS	Cross Section Information Storage & Retrieval System	Cross Section Information Storage & Retrieval System
ENDF	Evaluated Nuclear Data File (reaction)	McLane (1996)
ENSDF	Evaluated Nuclear Structure Data File	Tuli (2001),Winchell (2005)
EXFOR	EXchange FORmat, also see CSISRS	Cross Section Information Storage & Retrieval System
HTML	Hyper Text Markup Language	
HTTP	Hyper Text Transfer Protocol	
JEFF	Joint Evaluated Fission & Fusion file	Jacqmin et al. (2002)

(*continued on next page*)

Appendix 1 (*continued*)

Term or Acronym	Description	Reference
JENDL	Japanese Evaluated Nuclear Data Library (reaction)	Shibata et al. (2002)
JSP	Java Server Pages	Bergsten (2002)
MIRD	Medical Internal Radiation Dose	Medical Internal Radiation Dose
Mod_jk	Apache – Tomcat connector	The Apache Jakarta project
NRDC	Nuclear Reaction Data Centers network	Nichols (2005)
NSDD	Nuclear Structure and Decay Data evaluators network	Nichols (2005)
NSR	Nuclear Science References	Winchell (2005)
NuDat	Nuclear structure & decay Data	Sonzogni (2005)
RDBMS	Relational Database Management System	Lorents and Morgan (1998)
SQL	Structured Query Language	Lorents and Morgan (1998)
Sybase	Commercial database server	Sybase, Inc.,Rankins et al. (1996)
Tomcat	Servlet/JSP container	The Apache Jakarta project
USNDP	United States Nuclear Data Program	United States Nuclear Data Program (USNDP)
XUNDL	eXperimental Unevaluated Nuclear Data List	McMaster University Data Evaluation

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