National Nuclear Data Center
Report to the 2003 US Nuclear Data Program Meeting

P. Oblozinsky *et al*. (October 17, 2003)

The report summarizes activities of the NNDC for the period of April 1, 2002- September 30, 2003.

1. NNDC Operations

Personnel Changes

Since the last meeting of the US Nuclear Data Program, several personnel changes have taken place at the NNDC. Judy Tallarine (support staff, NSR bibliography compilation) retired in August 2002 and was replaced by Joann Totans. Ivan Sirakov (scientist, CSISRS compilation and ENDF management) completed his term in September 2002. Mike Herman was hired on March 1, 2003, with primary responsibility in nuclear reaction data evaluation and ENDF management. Boris Peterson (scientist, database application development) was hired on September 15, 2003 as replacement for Yako Sanborn (professional, system and database administration) who will retire on October 31, 2003. Sue Cataldo (administrative support) left on September 30, 2003; she will be replaced by Gail Brown (admin support, part time). With these changes, by the end of October 2003, the staff of the NNDC will be reduced to 12.25 FTE, including 8.0 full-time scientists, 1.75 professionals and 2.5 support staff.

Coordination and Reporting

We continue to provide secretariat functions and chair for the US Nuclear Data Program (USNDP) and for the US Cross Section Evaluation Working Group (CSEWG). In December 2002, the final report on the accomplishments of the Nuclear Data Program for FY 2002 was completed and distributed. The Workplan for fiscal year 2004 was completed and distributed in March 2003. Both of these documents were completed with the assistance of the Coordinating Committee of the USNDP. NNDC coordinated preparations for the USNDP Budget Briefing for FY 2005. The briefing was held at DOE, Germantown on March 13, 2003. Preparations started for issuing Workplan 2005.

Computer Support

The main work of the NNDC continues to be performed on our HP AlphaServer 4100. The nuclear databases reside on this computer and the related analysis, maintenance, or dissemination programs run on it. Due to the inherently more secure operating system on this computer (OpenVMS), we have been able to provide data services to external users while complying with the strict cyber security requirements of DOE. (Sanborn, Arcilla)

To support Database Migration Project described below, we operate several Linux servers. This includes Sybase ASE 12.5 primary and secondary database servers and data dissemination testing environment (working server). The working server will eventually replace the HP AlphaServer 4100 once the project is completed.

In March 2003, DOE approved capital funds for upgrading NNDC's aging computing infrastructure. The upgrade would be implemented in three phases and is already underway. In the first phase, we replaced the Linux working server with a dual-processor DELL server and connected to it a high-capacity tape drive to centrally backup all Linux servers and clients. In the second phase, we purchased another dual-processor DELL server to become our official, publicly accessible Web server. In the third phase (November 2003), we will replace our primary and secondary database servers with more modern and powerful servers. (Arcilla, Sanborn)

The above-mentioned DOE capital funds also allowed NNDC to purchase another high-capacity tape drive to centrally backup all Windows clients and servers. This more efficient backup strategy provides better protection for the staff's mission-critical data and codes from catastrophic system failures.

As part of its continuing effort to improve its staff's desktop computing capability, NNDC replaced nine PC's running on 466-MHz Intel Celeron with PC's having Intel Pentium 4 processors. An additional Intel Pentium 4-based workstation was purchased for M. Herman, NNDC's new staff member, to handle compute-intensive activities. NNDC staff use desktop PC's running Windows 2000, Windows XP or Red Hat Linux, depending on which operating system best suits the staff's task at hand. We also maintain Windows 2000 and Linux servers to meet NNDC's other computing needs.

2. Nuclear Database Migration

Previously, the NNDC has purchased and installed the Sybase Adaptive Server Enterprise (ASE) software on a Linux server. Relational versions of the nuclear structure databases, NSR, ENSDF, NuDat, and the reaction databases, CINDA, CSISRS, ENDF are being developed for this platform. The migration requires the development of new software and the modification of legacy codes to work with Sybase database software under Linux.

The nuclear structure databases are in the final testing phase. All NSR administration has been done under Linux since the summer of 2003. We expect to be running all production activities with these databases under Linux by the end of January 2004. The effort on migration of the nuclear reaction databases continues. This work should be completed in the fall of 2004.

In January 2004, our current Linux database server will be replaced by a state-of-the-art server and the databases moved to that computer. This computer will become the primary database server. A second, identical computer will be installed at the same time. A copy of the databases on the primary server will be maintained on this server and updated on a regular basis. This

secondary database server will serve the USNDP nuclear data to users outside of BNL through the BNL firewall. In this manner, we can isolate our internal maintenance activities from external access. In addition to hosting the master nuclear databases, the primary server will serve as 'warm standby' in case of failure of the secondary database server.

For Web-based retrieval of the data, we will be using Java Server Pages (JSP) hosted on a third Linux server, www.nndc.bnl.gov, located outside of the BNL security firewall. Data will be passed to this computer from the secondary database server via a tunnel through this firewall. On successful completion of the migration project, the NNDC online service (telnet) and the ALPHA 4100 computer will be retired.

3. Nuclear Structure Data

Evaluations. The following A-chain evaluations were completed: A=82 (Tuli), 138 (Sonzogni). The following nuclides were evaluated: ^{132,133,134}In, ^{140}Dy, ^{142}Ho (Sonzogni), ^{70}Ni, ^{78}Y, ^{78}Sr, ^{80}Y, ^{129}Ag, ^{140}Xe and ^{145}Sm (Tuli). Since the last meeting A=68 (Burrows), 82 (Tuli), 138 (Sonzogni) have been published. All nuclides submitted (Tuli, Sonzogni) were added to ENSDF. A=60 (Tuli), 134 (Sonzogni) have been submitted for publication.

Nuclear Data Sheets. In 2002, eleven issues of Nuclear Data Sheets consisting of ENSDF evaluation have been edited, prepared and sent to Academic Press for publication (Blennau, Tuli). The twelfth issue consisting of NSR updates was prepared and sent to Academic Press. In 2003, the work continued in a similar pattern (Tallarine/Totans, Winchell).

ENSDF and NuDat. The Evaluated Nuclear Structure Data File, ENSDF, has been continuously updated and maintained (Tuli) during the past year. The contents of the database have been distributed to the network in March, August, December 2002 and August 2003 (Tuli). NuDat has been updated following each distribution (Tuli).

Nuclear Wallet Cards. In March 2002, the DOE Security Office, Nuclear Materials Management and Safeguards System adopted the PDF version (January 2000) of Nuclear Wallet Cards as its official decay data standards. The standard is important for proper determination of amount of sensitive nuclear materials.

The Wallet Cards file has been updated, following ENSDF distributions; last update in August 2003 (Tuli).

ENSDF Analysis and Utility Codes. The ENSDF analysis and utility codes are maintained and upgraded (Burrows, Dunford). The current status of these codes will be available on the Web prior to the USNDP meeting.

Nuclear Science References. In FY02, altogether 4512 new references were added to NSR, 3276 with keywords. In FY03, 3673 references were entered, 2803 with keywords. Distributions of new and updated entries were carried out on a monthly basis.

Other Activities. T.W. Burrows and J.K. Tuli lectured for one week in November 2002 at the NSDD Evaluators' Training Workshop sponsored by the IAEA.

4. Nuclear Reaction Data

Database Codes

The NNDC continues to provide updates of CINDA, CSISRS and ENDF related codes to the following data centers: NDS, IAEA Vienna, VNIIEF Sarov, Russia, and the CNDC Beijing, China. (McLane)

Viktor Zerkin of the Nuclear Data Section (NDS), IAEA Vienna has made two visits to the NNDC, each for two weeks, and V. McLane visited the NDS for one week to discuss the design of a new relational nuclear reaction database.

Version 6.13 of the ENDF Utility codes described in last year's report has being released. Graphical input interfaces have been included in the UNIX and Windows versions of CHECKR, FIZCON, PSYCHE, STANEF and INTER. (Dunford)

CSISRS Compilation and ENDF Management

CSISRS Compilation. The compilation of experimental neutron and charged-particle reaction data into CSISRS database continued. In FY2002, the NNDC compiled neutron and charged-particle reaction data from 153 references. In FY2003, the NNDC compiled 42 neutron and 54 charged-particle reaction data sets. As of September 30, 2003, the NNDC has entered charged-particle reaction data from 1079 references measured in the U.S. and Canada (compare with 975 references reported in March 30, 2001). The CSISRS database now contains 1.15 million data points for charged-particle reactions, about 5.8 million data points for neutron reactions, and about 7.1 million data points for all reactions including photonuclear reactions. (McLane)

ENDF Management. The management focused on work related to development of new version of the library, ENDF/B-VII. An extensive Preliminary ENDF/B-VII Web page was set up for new and revised evaluations, including easy access to files, results of checking codes, and numerous intercomparison plots to facilitate reviewing process. As an example, we show in Fig.1 the initial part of the information with numerous links for more details on new evaluation for ^{99}Tc. The related CSEWG Web page was updated. (Herman, Oblozinsky)

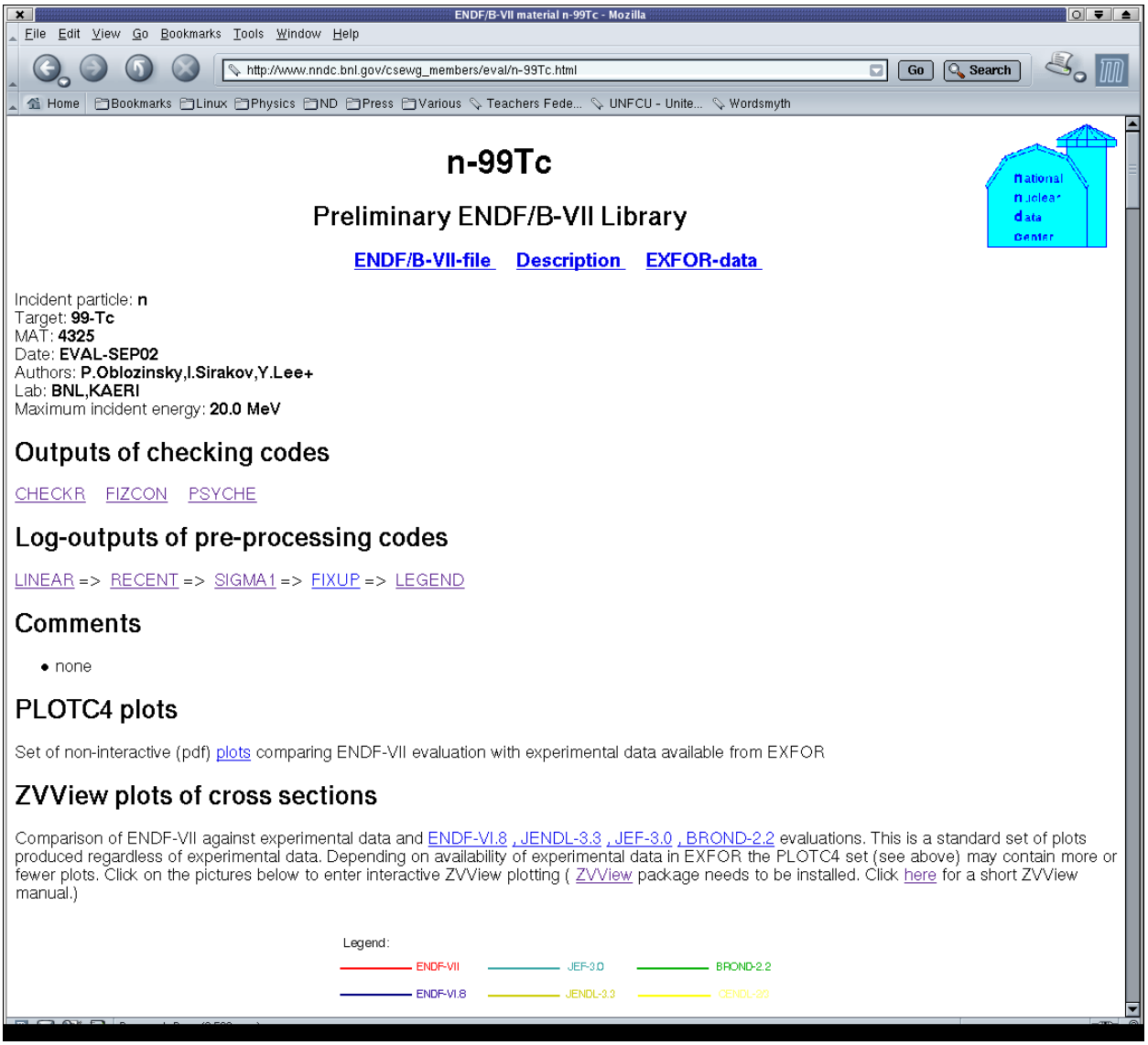


Fig. 1. Preliminary ENDF/B-VII Web page: Example of information provided for new evaluation. Not shown are numerous intercomparison plots.

Evaluation

Model Code Development. Collaboration with LANL (Chadwick) and IAEA Vienna (Trkov and Zerkin) on the development of a modular nuclear reaction model code EMPIRE (principle author M. Herman) for nuclear reaction data evaluations continued. Validation of the Monte Carlo Hybrid Monte Carlo code DDHMS (authors M. Chadwick and M. Blann, LANL) was performed using extensive set of about 150 nucleon induced reactions on 35 target nuclei, focusing on incident energies 10, 14 and 26 MeV. Several improvements of the code EMPIRE were done, including new graphic user interface shown in Fig. 2, merging of resonance and fast energy region into single ENDF-6 file, and plotting of particle spectra and angular distributions. (Herman, Oblozinsky)

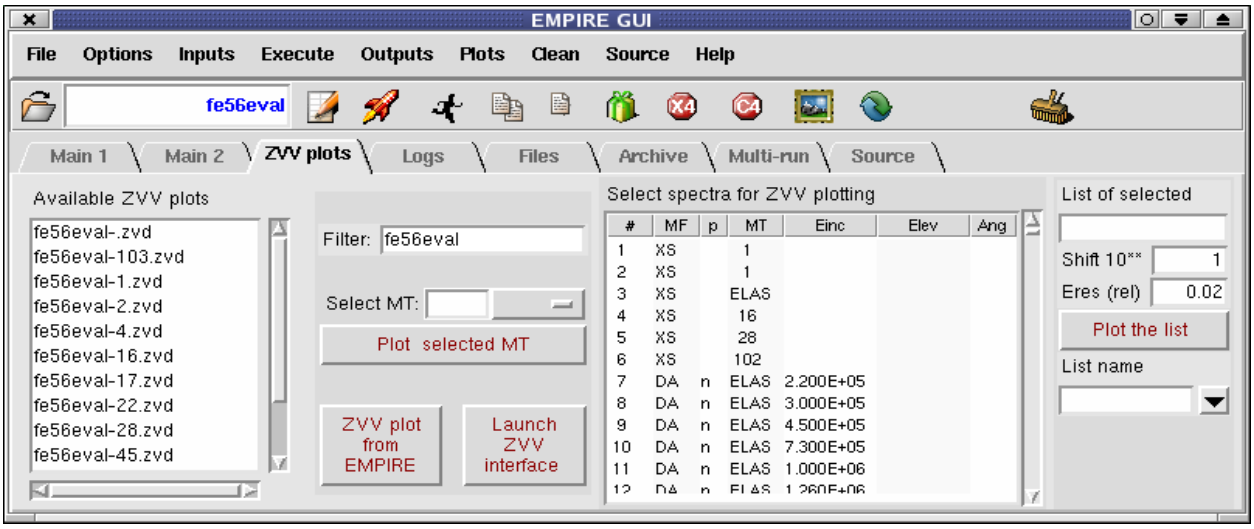


Fig. 2. Powerful graphic user interface developed for unreleased Empire-2.19 package. It provides extremely efficient way to run this complex code system, including access to associated data libraries, and multitude of utility codes such as ZVView used to produce ZVV plots.

Fission Products. Collaboration with the Korean Atomic Energy Research Institute (KAERI) on 19 fission product cross-section evaluations was completed and final files were prepared. Evaluations for 3 materials, ^{99}Tc, ^{153}Eu and ^{157}Gd, were submitted to ENDF/B-VII by the NNDC. Remaining materials, including 12 spherical nuclei, ^{109}Ag, ^{133}Cs, ^{95}Mo, ^{143,145}Nd, ^{105}Pd, ^{141}Pr, ^{103}Rh, ^{101}Ru, ^{147,149}Sm and ^{131}Xe, and 4 deformed nuclei, ^{149,50,151}Sm and ^{149}Gd were prepared by KAERI. In view of format problems in all KAERI files, these are being reformatted; afterwards they will be viewed as submitted to ENDF/B-VII. (Oblozinsky, Sirakov, Herman)

Reviews. Review of all available fission product cross sections from 5 international data files (ENDF/B, JEF, JENDL, BROND and CENDL) continued as an international project (NEA WPEC Subgroup 21, chaired by P. Oblozinsky). The project intends to review all 211 evaluations in the fission products region (Z = 31 - 68), to focus on the bulk of evaluations and to recommend the best evaluations for inclusion into ENDF/B-VII. After completion of trial reviews for 18 materials in 2001, SG21 reviewed another 89 materials including 20 by the NNDC. (Oblozinsky, Sirakov, Herman)

Homeland Security. Photonuclear data on ^{14}N were evaluated for 9.17 MeV resonance photons, to be used at BNL for MCNP simulations of the Gamma Resonance Technique to detect explosives. Preliminary evaluation of ^{74}Ge+n was performed with a focus on complete discrete and continuous photon production data that are needed for MCNP simulations of detector systems using Germanium. To validate EMPIRE procedures for gamma production, well-measured ^{56}Fe+n was compared with calculations shown in Fig. 3. In both instances, close collaboration with LANL was maintained. (Oblozinsky, Herman)

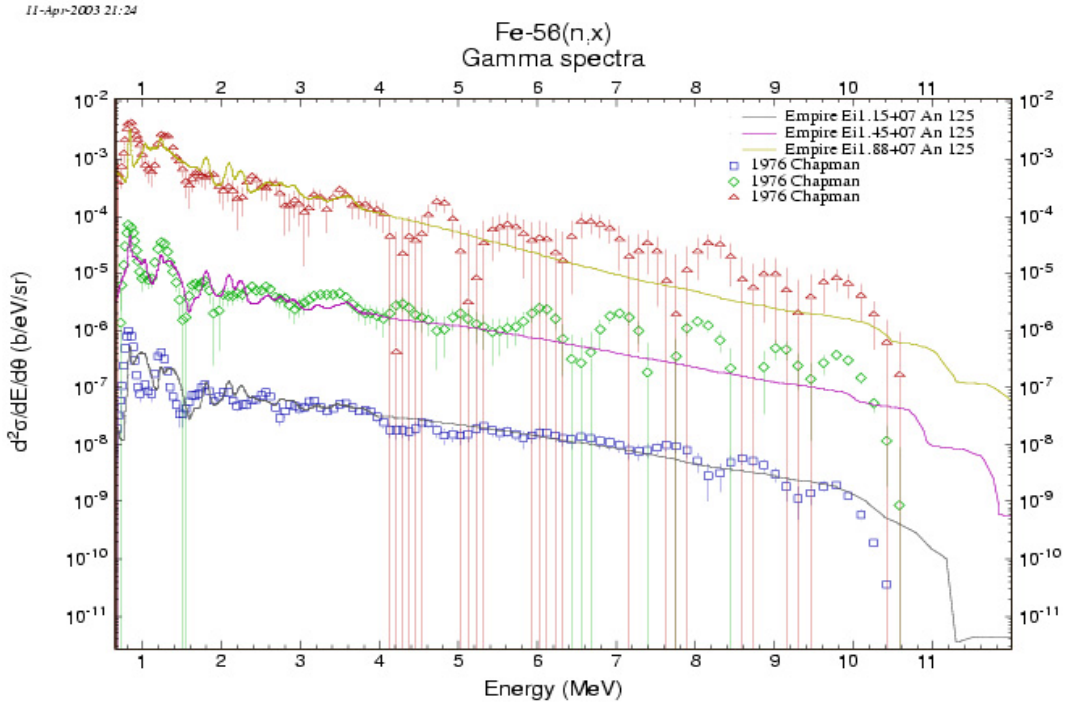


Fig. 3. Experimental gamma spectra from ^{56}Fe+n at E_n = 11.5, 14.5 and 18.8 MeV compared with ENDF-6 results provided by Empire-2.18. The code performed model calculations, followed by ENDF-6 formatting.

Other Activities

Victoria McLane and Pavel Oblozinsky attended the Nuclear Reactions Data Center Network Meeting, May 2002, Paris. Pavel Oblozinsky participated in the Workshop on the Role of the Nuclear Research Community in Combating Terrorism, July 2002, Washington, DC. Pavel Oblozinsky, Charlie Dunford and Mike Herman attended the WPEC annual meeting, May 2003, Coronado/San Diego.

The NNDC, in cooperation with Russian Nuclear Data Center VNIIEF, Russia, and Michael Smith (ORNL), has been awarded a grant from the Civilian Research and Development Foundation (CRDF) for the "Compilation and Evaluation of Alpha-Induced Nuclear Reaction Cross Sections for Astrophysics".

5. Data Dissemination

Internet

Internet access to the data and information available at the NNDC consists of:

1. Web (Arcilla, Blennau, Burrows, Dunford, McLane, Sanborn, Tuli, Winchell)
2. TELNET (Burrows, Dunford, McLane)
3. Anonymous FTP (Burrows, Dunford)

As shown in Fig. 4, there was about an 8% increase in the number of retrievals over the Internet between 2001 and 2002. The increase between FY2002 and FY2003 was 17.2%. NuDat and NSR continue to be the most popular with 25% and 24% of the 2002 retrievals, respectively. Retrievals from the nuclear reaction databases (CINDA, CSISRS, ENDF) accounted for 15% of the retrievals while retrievals from ENSDF, MIRD, and XUNDL amounted to 18%. Retrievals *via* the Web, including the NSR SQL Server accounted for about 94% of the total with approximately 6% and less than 1% *via* TELNET and anonymous FTP, respectively.

Strong usage of NSR link manager continued in 2002. In addition to NNDC pages, URL's using the manager include:

atom.kaeri.re.kr	radware.phy.ornl.gov	www-nds.iaea.org
www-nds.ipen.br	www.td.anl.gov	www.tunl.duke.edu
www.google.com	www.google.de	www.google.com.ru
www.google.com.fr	www.google.com.nl	yahoo.com
216.239		

The ENSDF Link Manager was not accessed in 2002.

Additions and Improvements

1. Balraj Singh's Table of Super-deformed Bands and Spontaneous Fission Isomers was added to the NNDC site.
2. Proceedings of the "CSEWG Symposium: A CSEWG Retrospective" added.
3. HTML forms and CGI-scripts for CINDA, ENDF, MIRD, and NuDat upgraded.
4. The ENDF Utility Codes Web and FTP sites were reorganized and Linux and MS Windows versions were added.
5. A Web interface to the NNDC OnLine Data Service Open Area was added.
6. Data Object Identifiers were added to NSR entries for Elsevier and EDP Sciences journals in the NSR SQL Server.
7. EXFOR Basics manual added.

Other Changes

1. The Codes, Documentation, and Data Libraries modules of the NNDC OnLine Data Service (TELNET) were removed.

Current Activities and Future Plans

The major effort is in converting the databases resident on the NNDC OpenVMS machines to Sybase relational databases on Linux or UNIX platforms and developing Web interfaces to the new databases using jsp (Java Server Pages) or Java servlets. These interfaces will have all the capabilities of the current TELNET and Web interfaces.

After the database conversions are completed and tested, the remaining portions of the NNDC Web site will be transferred. The NNDC will attempt to do this move in a manner that will be transparent to the users.

Hardcopies and CD-ROM

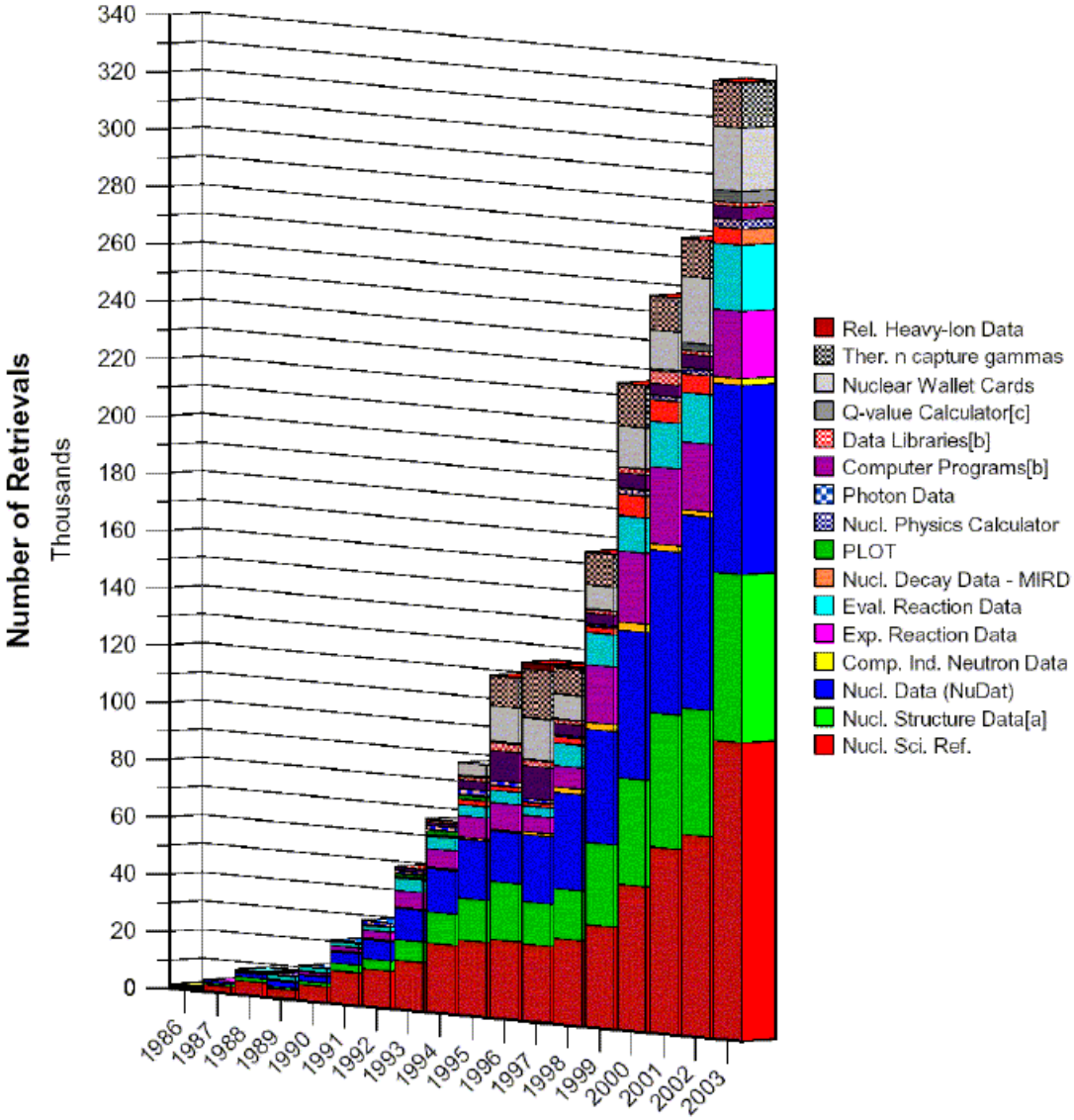
The *Nuclear Data Sheets* continue to be edited and produced by the NNDC for publication by Academic Press. The cost of this activity is fully covered by royalties and other payments received from Academic Press. Eleven issues are devoted to publication of ENSDF evaluations. The December issue is devoted to "Recent References" which are the yearly updates to Nuclear Science References. The journal is now available on the Elsevier Web sites but is no yet indexed in their Science Server. Starting with *Nuclear Data Sheets* **98** (2), the NNDC is providing the PDF directly to Academic Press. (M. Blennau, V. McLane, J. Tallarine/J. Totans, J.K. Tuli, D.F. Winchell)

The NNDC satisfied 2 requests for the PCNuDat database, 4 requests for ENDF, and 1 request for the ENDF Utility Codes on CD-ROM between March 15,2002 and April 2, 2003.

User Outreach

The NNDC continues to host the USNDP Web site, CSEWG Web site, and International Nuclear Structure and Decay Data Network Web site. The IAEA Nuclear Data Section has taken over maintenance of the Web site for the Nuclear Reaction Data Centers (NRDC) Network.

*NNDC On-Line Data Service, Web, & FTP Retrievals 1986-2003**



* Extrapolated as of September 30, 2003.
[a] Includes proton emitters (added to Web February 21, 2002).
[b] Removed from Online Data Services June 25, 2002.
[c] Added to Web September 11, 2001.

Fig. 4. Data Retrievals (1986-2003)