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Nuclear Data Resources for Advanced Analysis and Simulation

B. Pritychenko

National Nuclear Data Center, Brookhaven National Laboratory
Upton, NY 11973-5000, U.S.A.

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Energy Science & Technology Department
National Nuclear Data Center
Brookhaven National Laboratory
P.O. Box 5000
Upton, NY 11973-5000
www.bnl.gov

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B. Pritychenko[1]

National Nuclear Data Center, Brookhaven National Laboratory
Upton, NY 11973-5000, U.S.A.

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. Examples of nuclear reaction, nuclear structure and decay database applications along with a number of nuclear science codes are also presented.
KEYWORDS: Nuclear Reactions, Nuclear Data Dissemination, Nuclear Data Analysis

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 [1]. The NNDC mission includes collection, evaluation, and dissemination of nuclear physics data for basic nuclear research and applied nuclear technologies [1-3].

The NNDC maintains and contributes to the nuclear reaction (ENDF, CSISRS) and nuclear structure databases along with several other databases (CapGam, MIRD, IRDF-2002) and provides coordination for the Cross Section Evaluation Working Group (CSEWG) and the US Nuclear Data Program (USNDP). The Center produces several publications such as Atlas of Neutron Resonances [4] formerly known as BNL-325, Nuclear Wallet Cards booklets [5,6] and develops codes, such as nuclear reaction model code Empire [7].

2. NNDC Computer Environment

The NNDC has been providing remote electronic access to its databases and other information since 1986. In order to improve the quality of nuclear data services and take advantage of latest software and hardware developments, NNDC started a nuclear database migration project in 1999.

New Web interfaces integrated with relational databases created a Nuclear Data Portal http://www.nndc.bnl.gov that was launched on April 19, 2004 [3]. 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

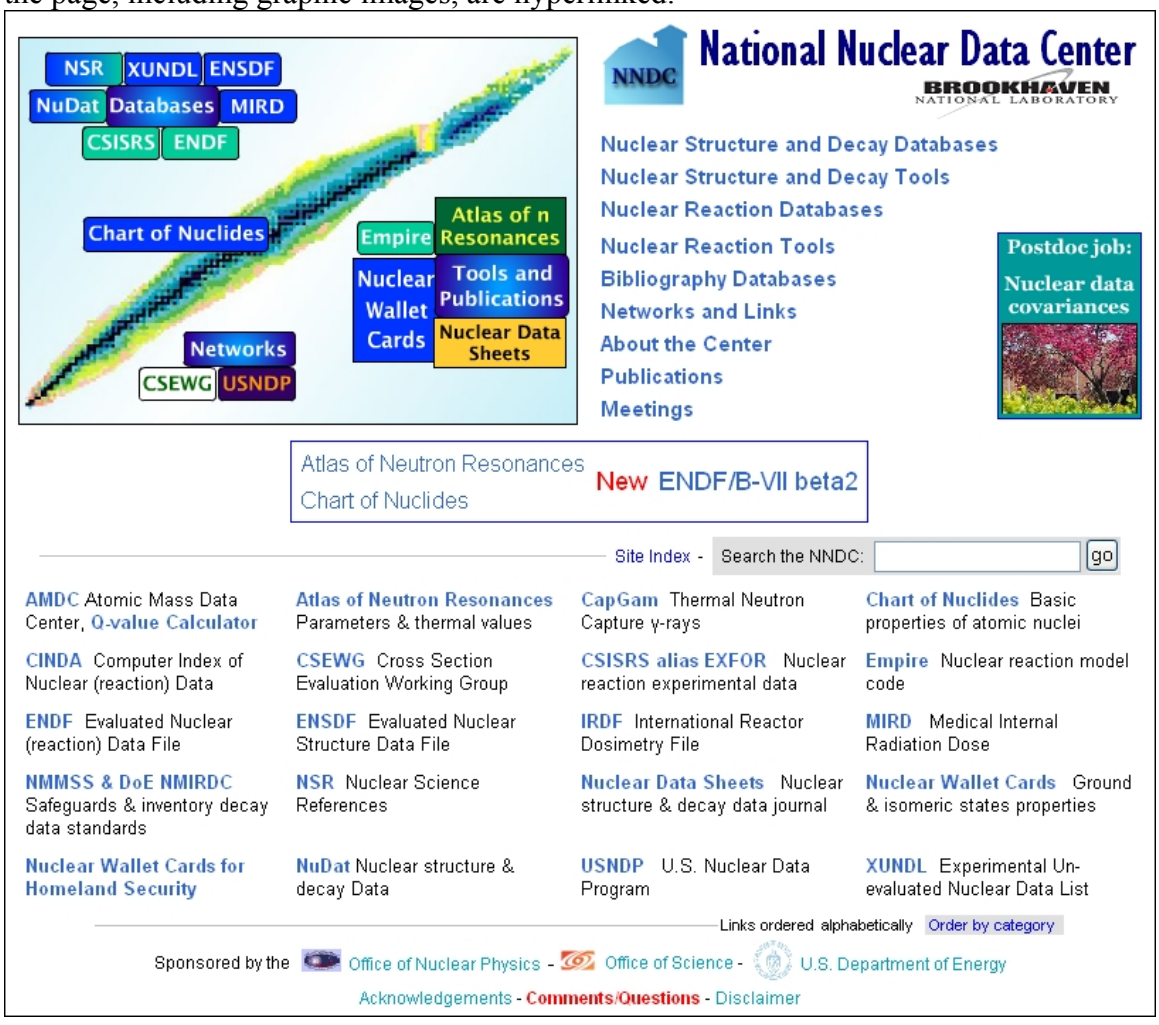
[1] Corresponding author, Tel. 631-344-5091, Fax. 631-344-2806, E-mail: pritychenko@bnl.gov

reaction, decay and structure data, as well as bibliographical information. Its major features include:

- A new generation of nuclear data services using 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)
- A Google search engine and site index for NNDC documents
- Web interfaces for nuclear databases
- On-line query forms for information searches; results are presented in tables and interactive plots
- Numerous nuclear science tools, codes, applications, and links

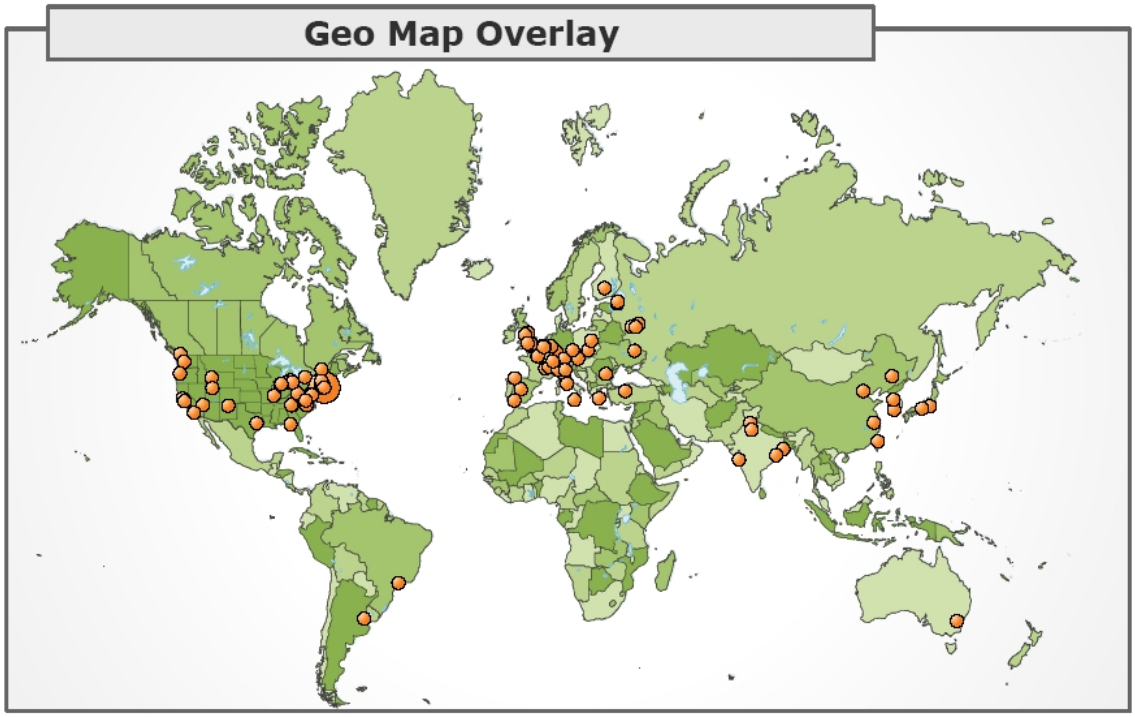
The new Web-based nuclear data retrieval system or Nuclear Data Portal is tightly integrated with nuclear reaction (CSEWG) and structure (USNDP) evaluations and compilation efforts. The portal is shown in Figure 1.

Figure 1. Front page of the NNDC Web Services (www.nndc.bnl.gov). All elements of the page, including graphic images, are hyperlinked.



The new Web-based nuclear data retrieval system generated overwhelming response from nuclear data users. This system produced a two-fold increase in the NNDC Web data retrievals compared with the previous service. Nuclear data users from more than 12000 organizations requested data from NNDC in 2005. Geographical distribution of nuclear data users is shown in Figure 2. If this trend continues, the forecast for FY 2006 will be over 900 K retrievals. It is expected that the NNDC nuclear data retrieval system will meet growing demands in the future.

Figure 2. Geographical distribution of nuclear data users, major nuclear data customers are from North America and Europe. This plot was produced by Google analytics (http://www.google.com/analytics).



3. Nuclear Databases

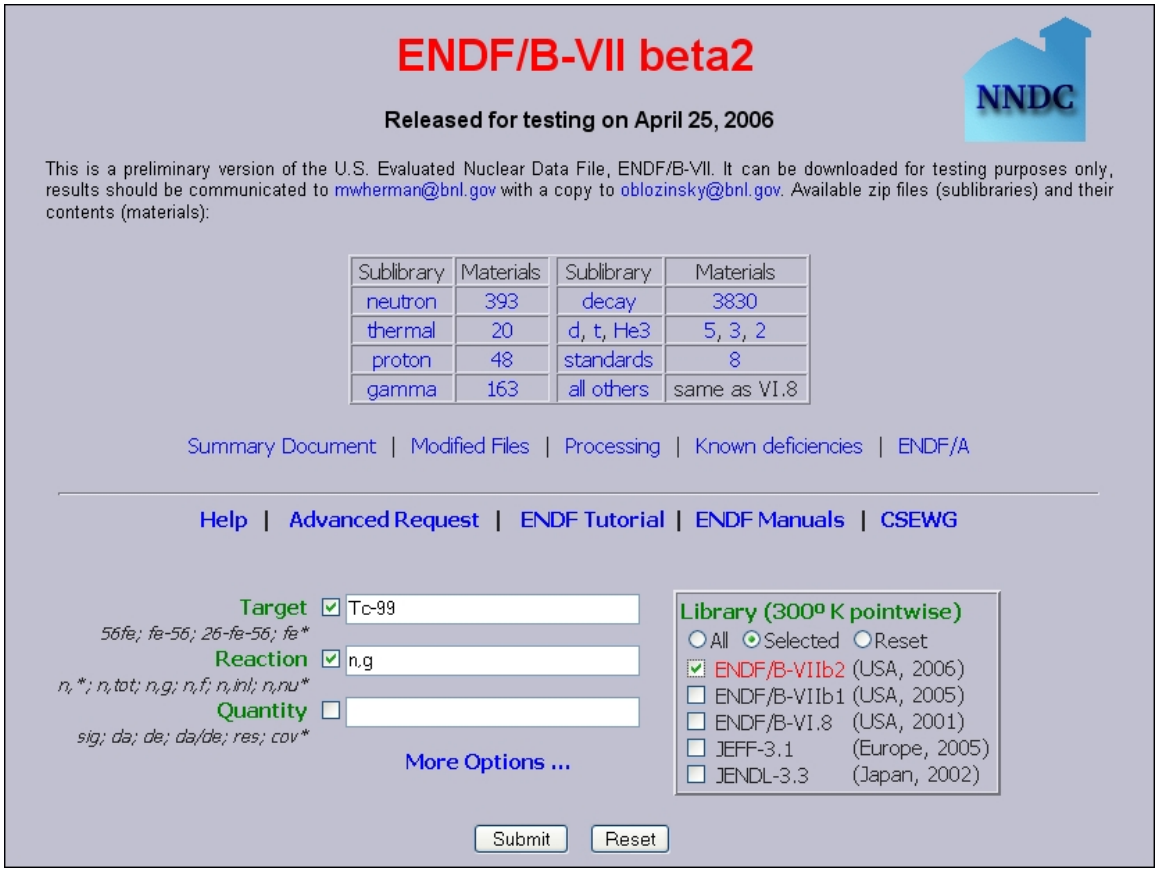
Nuclear data services were substantially improved to provide a better access to reaction data evaluations and compilations [2]. New Web interfaces for the Evaluated Nuclear Data File (ENDF) and the nuclear reaction experimental data (CSISRS/EXFOR) provide a wide range of options for data retrievals and analysis using standard and interpreted text formats as well as graphic tools. New nuclear reaction services differentiate themselves by the simple manner of creating on-line database queries and the extensive use of graphics. A brief description of the nuclear databases is presented below.

3.1 Evaluated Nuclear (reaction) Data File

The ENDF reaction database contains recommended data from the United States ENDF/B-VI.8 library. ENDF Web interface also provides access to the other evaluated nuclear reaction libraries: JEFF-3.1, JENDL-3.3, BROND, and CENDL.

At the present time, the ENDF nuclear reaction database is under new development. ENDF/B-VII library verification includes ENDF checking codes: CHECKR, FIZCON, PSYCHE, STANEF and the processing of data files with NJOY-99.124 and Monte Carlo Neutron Transport (MCNP) codes. Checking codes, NJOY and MCNP are used to verify that all evaluated data are confirmed to ENDF-6 format. ERRORJ is used for processing the new covariance data. Processed files are loaded into the Sybase relational database and are accessible on Web. The latest version of the library, ENDF/B-VII beta2 was released on April 25, 2006 by CSEWG. Web interface for ENDF/B-VII beta2 is shown in Figure 3.

Figure 3. ENDF/B-VII beta2 Web interface (http://www.nndc.bnl.gov/endf2).

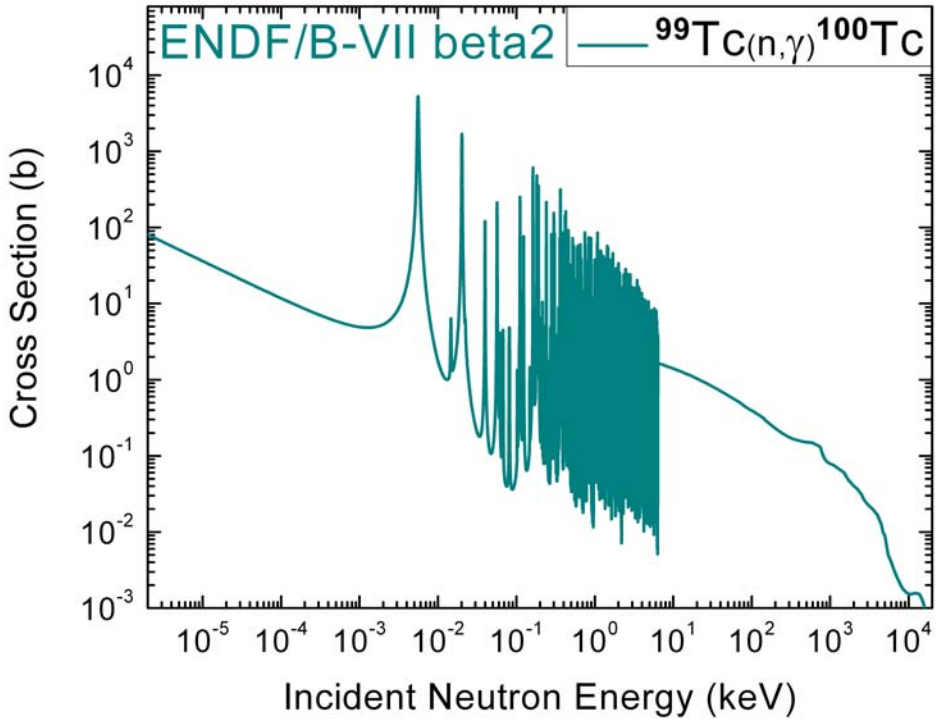


Currently developed and extensively tested ENDF/B-VII beta2 library and corresponding Web service www.nndc.bnl.gov/endf2 contain neutron cross sections for

393 materials relevant to nuclear technology. This library also includes 8 nuclear data standards, 20 thermal scattering, 48 proton, 163 photo-nuclear, 3830 decay and 10 charged-particle evaluations.

Figure 4 shows a new ENDF/B-VII evaluation of an important fission product ^{99}Tc. ^{99}Tc(n,γ)^{100}Tc reaction is important due to a relatively large neutron absorption cross section that restricts life-time of the fuel rods and transmutation of nuclear waste. The latest evaluation of ^{99}Tc was performed at the National Nuclear Data Center by P. Oblozinsky, D. Rochman, M. Herman and S. Mughabghab [2]. We expect that a final version of ENDF/B-VII library and a new Web application will be available in 2006.

Figure 4. Evaluated cross section for ^{99}Tc(n,γ)^{100}Tc reaction. This reaction is important in reactor physics and radioactive waste transmutation.

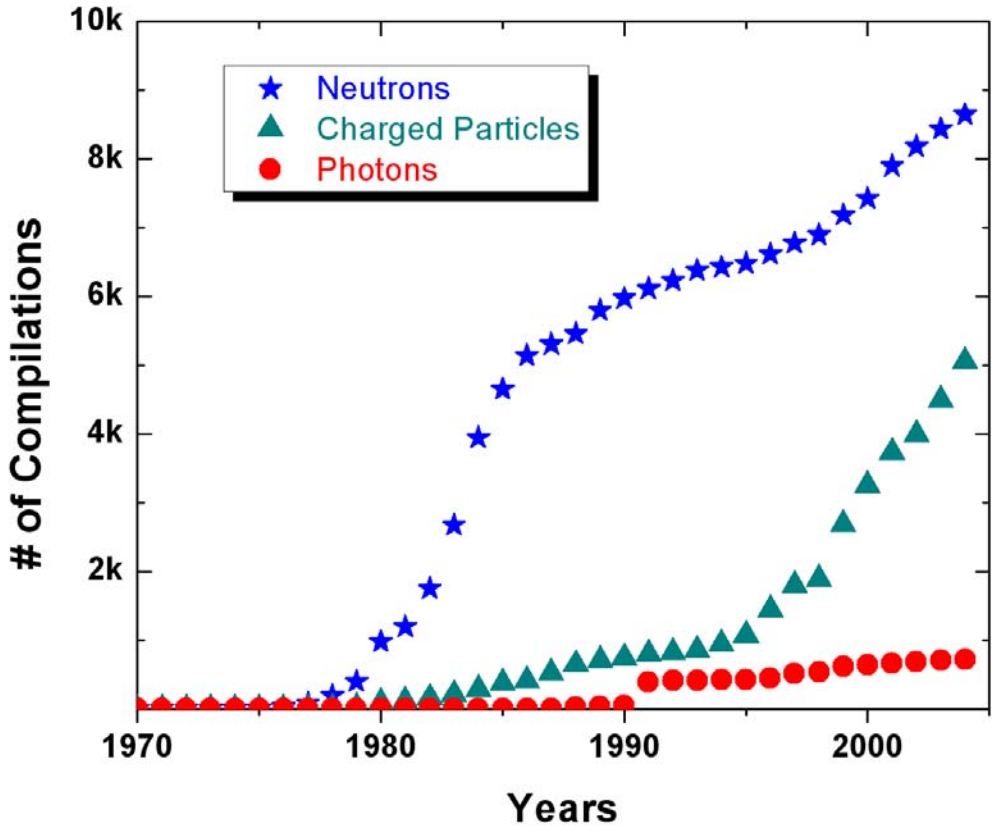


3.2 Experimental Nuclear Reaction Data

Cross Section Information Storage & Retrieval System (CSISRS), alias EXFOR (EXchange FORmat) data library [1-3] contains experimental nuclear reaction data for incident neutrons, charged particles, and photons. It includes more than 15500 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 < 12) and photon experiments. Figure 5 indicates that in the recent years the

number of charged particles compilations is increasing faster than others. The content of the CSISRS database, serves as a principal input for ENDF nuclear data evaluations.

Figure 5. Compilations of nuclear reaction experimental data into CSISRS database over the last 30 years



3.3 Other Databases

The thermal neutron capture γ-ray database (http://www.nndc.bnl.gov/capgam) provides energies and intensities of γ-rays for nuclear reactor heat calculations. CapGam database contains thermal neutron capture γ-ray information on 256 target nuclides of interest up to 12 MeV in energy. Database content, produced from the Evaluated Nuclear Structure Data File (ENSDF), is searchable by isotope or γ-ray energy.

Medical Internal Radiation Dose database (http://www.nndc.bnl.gov/mird) contains recommended nuclear decay data for over 2100 radionuclides extracted from ENSDF, processed by the program RadList and presented in the Medical Internal

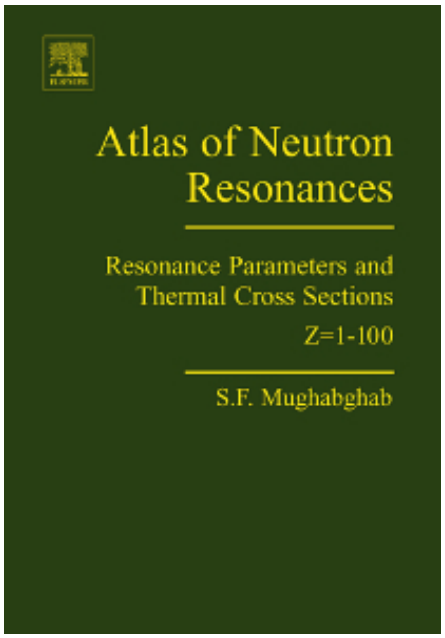
Radiation Dose format.

The International Reactor Dosimetry File: IRDF-2002 is a standardized, updated, and benchmarked evaluated cross section library of neutron dosimetry reactions with uncertainty information for use in lifetime management assessments of nuclear power reactors and other neutron metrology applications such as boron neutron capture therapy, therapeutic use of medical isotopes, nuclear physics measurements, and reactor safety applications (http://www.nndc.bnl.gov/nndcscr/libraries/irdf/).

4. Publications & Codes

Atlas of Neutron Resonances reference book (http://www.nndc.bnl.gov/atlas/) represents the 5th edition of BNL-325 and was published by Elsevier on April 17, 2006 [4]. It contains evaluated neutron data for 98 elements and 486 ground and isomeric states of 476 isotopes (381 isotopes with resonance data) and represents one of the most comprehensive thermal, resonance, and unresolved energy region neutron data resources. All nuclear data evaluations and compilations were conducted at the National Nuclear Data Center, Brookhaven National Laboratory. The front page of Atlas of Neutron Resonances is shown in Figure 6.

Figure 6. The cover of Atlas of Neutron Resonances reference book [4].



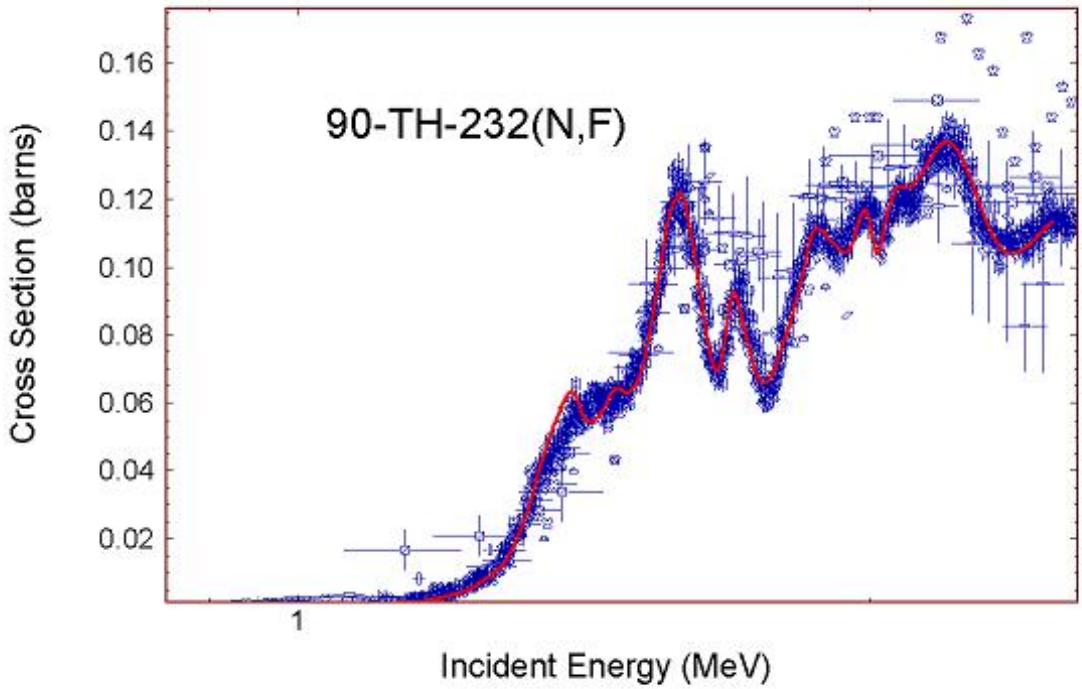
The Nuclear Wallet Cards publication, currently in its seventh edition, contains up-to-date information on 5657 ground and isomeric states properties of all known

nuclides (http:// www.nndc.bnl.gov/wallet). The sixth edition of Nuclear Wallet Cards [5] has been adopted by the U.S. Department of Energy, Nuclear Materials and Safeguards System as their decay data standard.

A version tailored for Homeland Security needs is also available [6]. Nuclear Wallet Cards for Radioactive Nuclides include nuclear properties of $T_{1/2}$ <= ~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.

EMPIRE (http:// www.nndc.bnl.gov/empire) is a modular nuclear reaction code for advanced calculation of nuclear reactions using various theoretical models [7]. It consists of a number of linked FORTRAN codes, input parameter libraries, and the experimental data library (CSISRS/EXFOR). Figure 7 demonstrates Empire 2.19 code capability of reproducing complicated structure in the fission cross section.

Figure 7. Empire 2.19 results for neutron-induced fission of ^{232}Th compared with experimental data [7].



5. Conclusion and Outlook

Nuclear data resources of the National Nuclear Data Center (NNDC) of relevance to nuclear industry, as well as, applied technology applications were discussed. These resources include databases, tools, publications and powerful Web service at http://www.nndc.bnl.gov. A successful completion of the nuclear database migration project [3] brings confidence that NNDC has considerable potential to meet growing demands in the coming years.

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