

STATUS AND PERSPECTIVE OF NUCLEAR DATA PRODUCTION, EVALUATION AND VALIDATION

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A very important feature in the development of nuclear technology has been and will continue to be the flow of information from nuclear data production to the various applications fields in nuclear technology. Both, nuclear data and this communications flow are defined in this paper. Nuclear data result from specific technical activities including their production, evaluation, processing, verification, validation and applications. These activities are described, focusing on nuclear reactor calculations. Mathematical definitions of different types of nuclear data are introduced, and international forums involved in nuclear data activities are listed. Electronic links to various sources of information available on the web are specified, whenever possible.

1. INTRODUCTION

Nuclear data are physical parameters that describe the internal structure of nuclei, their decay and interactions with incident particles. They include:

- Atomic and molecular data.
- Nuclear reaction data.
- Nuclear structure and decay data.

Atomic and molecular data are included in a broad sense because of their relevance to a full description of the interactions, production and transport of particles. Nuclear structure and decay data are important for the development of theoretical nuclear models, with which the properties of nuclei interacting with other particles can be described. Nuclear reaction data are the primary topic of review in the present work, with special emphasis on neutron-induced interactions.

Reaction rates of neutron interactions with matter are the key parameters of interest in nuclear applications such as reactor core design calculations, shielding problems, activation, burnup, etc. They are parameterised by the neutron flux (that describes neutron population) and nuclear reaction data (which define the properties of the medium). Reaction rates determine most other parameters of interest, like the neutron fluence in shielding problems, multiplication factor and power distribution in nuclear reactors, etc. Consider for example a nuclear reactor core design calculation. The neutron multiplication factor and the neutron flux distribution under various operating conditions need to be calculated repeatedly. A long chain of calculations needs to be performed, with

input parameters that describe the geometry, material composition and the *neutron nuclear reaction data* (i.e. the cross sections, their energy dependence, energy spectra and angular distributions of secondary particles etc. for all nuclides of each material that constitutes the reactor core assembly). For shielding calculations the same data are used, except that in addition, photon interaction and coupled neutron-photon and charged-particle interaction data are sometimes required.

Nuclear data are needed in a variety of applications: they facilitate the development of advanced analytical techniques in medical diagnostics and therapy, geological prospecting, environmental monitoring, detection of explosive devices, as well as nuclear power utilisation. It is true that early nuclear reactor concepts were designed successfully without the wealth of information available today. However, the designers required small experimental facilities on which they measured integral parameters and extrapolated them as required during the design of the full-scale facility. Flexibility in the design characteristics was limited to those that could be verified in the experimental facilities. Nowadays, availability of basic nuclear data allows design optimisation by computational models, thus greatly reducing the need for expensive experimental facilities, except for design concept verification in the final stages of the design process.

The main objective of the present work is to describe the flow of information from basic nuclear data production to advanced applications in nuclear technology, to present various international forums

involved in nuclear data activities, and to provide an overview that might help the reader to locate the most convenient sources of information for applications in nuclear technologies.

2. OVERVIEW

At the Geneva Conference in 1955 an international agreement was reached to stimulate free and open exchange of nuclear data, in order to support the growth of the peaceful applications of nuclear energy. The circumstances were ripe for the establishment of the International Atomic Energy Agency in 1957 and the Agency's Nuclear Data Programme started in 1963.

The field of nuclear data development is a rare example of a case in which international collaboration has been intense and continuous over a period of several decades. As the amount of exchanged experimental data was increasing, there was a need for computerised data management. The EXFOR Agreement on the format for storing experimental data was reached at a meeting in Moscow in 1969. The data centres at Brookhaven serving USA and Canada, Obninsk serving the former Soviet Union, Paris serving Europe and Japan and the IAEA in Vienna serving the rest of the Member States, took the responsibility to compile and exchange published experimental data in computerised format. As a result of these combined efforts an enormous wealth of knowledge has been accumulated and is available without restrictions to all potential users. Apart from national projects, intergovernmental agencies such as the International Atomic Energy Agency (IAEA) and the Nuclear Energy Agency (NEA) of the Organisation for Economic Co-operation and Development (OECD) provide natural environments for the co-ordination of data development activities. A good example is the OECD/NEA Working Party on Evaluation Co-operation (WPEC), which provides a forum for the exchange of information on the activities and programmes of national projects, and organises Sub-groups that jointly address burning issues of mutual interest. Details about the past and currently-active Subgroups are available on the WPEC web site <http://www.nea.fr/html/science/wpec/index.html>. Similarly, the mechanism of Co-ordinated Research Projects (CRP) of the IAEA plays an important role by facilitating scientists from the Member States to participate in data development projects. Details can be found on the web site of Nuclear Data Section of the IAEA at <http://www.naweb.iaea.org/naweb/nd/index.asp>.

3. CLASSIFICATION AND DEFINITIONS

Nuclear reaction data for individual isotopes at particular energies of incident particle can be measured

experimentally, or else they are predicted by nuclear model calculations. Usually an experiment provides a single parameter value (i.e. cross section at a particular energy) or at most, the cross section behaviour over a rather limited energy range. For each reaction the cross sections are strongly energy dependent and rather difficult to model or predict analytically from first principles. Also, in a realistic situation, one needs to consider a mixture of a number of materials. Therefore, the necessary amount of information increases enormously. This immediately raises the following points:

- In order to obtain sufficient data, a very large number of experiments must be performed. International collaboration and data exchange are essential.
- Since the amount of data is large, it must be presented in computer-readable form.
- When no experimental data in a certain energy range exist, one must resort to theoretical model calculations and the systematics (if any) in the cross-section behaviour of nuclei with similar characteristics (i.e. similar parity in the number of neutrons and protons, etc.).
- When more than one measurement exist for a quantity, each measured with a certain error, an evaluation is necessary to obtain the "best estimate" value.
- Routinely used computer codes for solving reactor core and shielding problems appear in iterative procedures and computation time is crucial. For this reason the full details of the energy dependence of parameters are not taken into account. Data reduction techniques are necessary.

In view of the discussion above, the following tasks associated with the nuclear data can be identified:

- production (measurements and theoretical calculations),
- evaluation,
- processing,
- verification,
- validation and benchmarking,
- applications.

The flow of information is displayed schematically in Figure 1.

Depending on how the data are obtained and for what purpose they are used, the following categories of nuclear data can be identified:

- **Basic experimentally measured nuclear data** : refer to quantities like half-lives, cross sections measured at a specific incident particle energy or differential cross sections measured at specific incident particle energy, outgoing particle energy and angle, etc.
- **Integral experimentally measured data** : refer to parameters that can be defined from the basic nuclear data as sums, products, quotients, integrals, etc. They

can be simple, spectrum-averaged cross sections, resonance integrals, or more complex quantities like the multiplication factor of a reactor lattice.

- **Evaluated nuclear data** : refer to the result of the process whereby the basic experimentally-measured nuclear data are reviewed, analysed by statistical methods (when several measurements for the same quantity are available), supplemented by theoretical model calculations and assembled into evaluated

nuclear data files in specific format. Such files serve as a starting point for the preparation of application libraries.

- **Processed nuclear data files** : may imply a simple change of representation of the data, Doppler broadening of resonances to account for temperature effects or complex averaging procedures resulting from data reduction techniques.

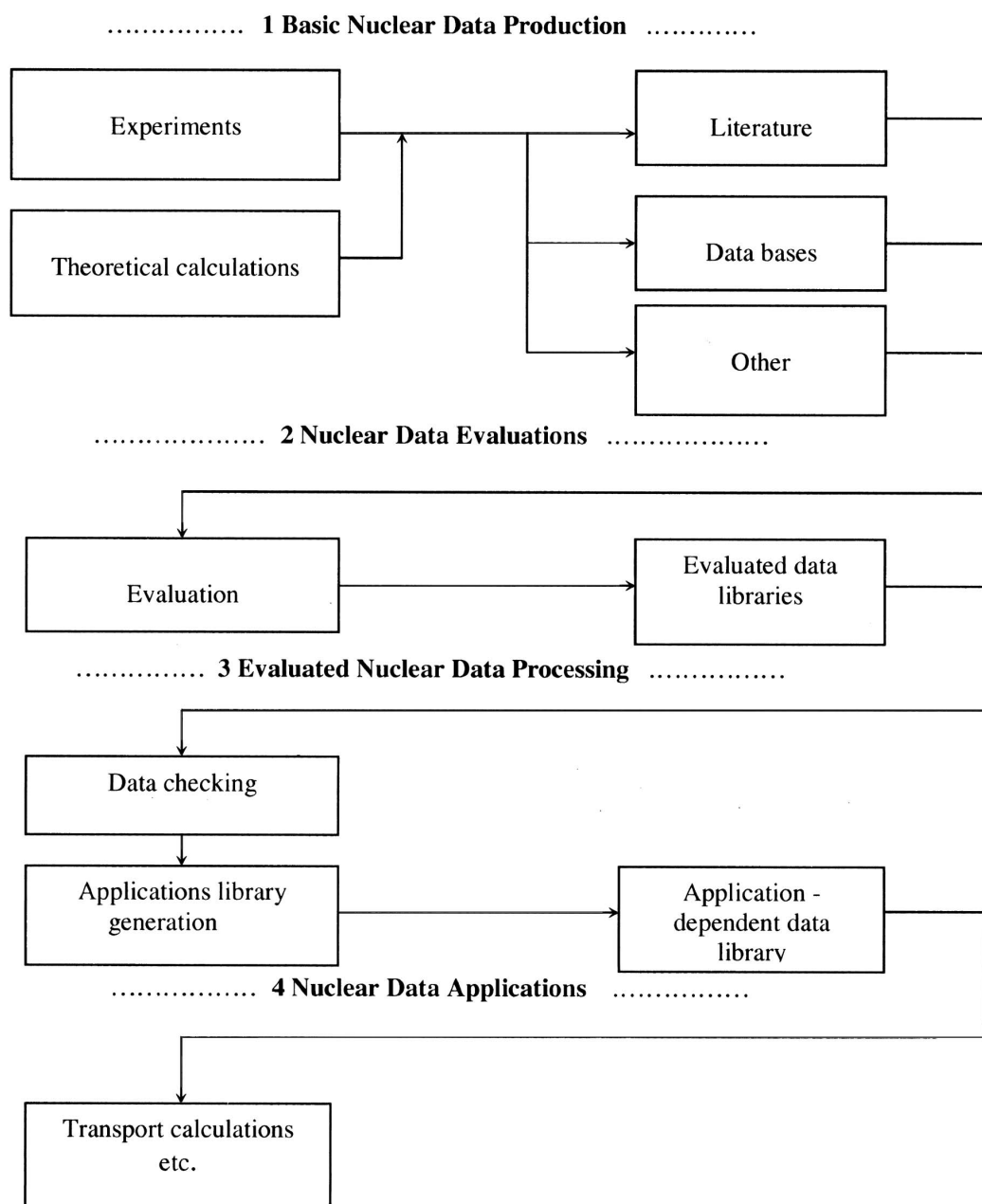


Fig. 1. Activities associated with Nuclear Data.

3.1 Nuclear Data Activities

3.1.1 Nuclear data production

Experimental measurements : In the past, *integral measurements* on reactor lattices were usually mock-up experiments, needed for the validation of design features of new facilities. Nowadays they serve for the validation of the computational tools and/or nuclear data. A large number of well-documented experiments of this type is available on the OECD/NEA server <http://www.nea.fr/html/dbprog/benchmarks.htm>, such as:

- ICSBEP International Handbook of Evaluated Criticality Safety Benchmark Experiments [1], focusing mainly on criticality.
- IRPhE International Reactor Physics Benchmark Experiments Project, containing a broader variety of measured integral constants [2].
- SINBAD Shielding Integral Benchmark and Database [3].

Other types of integral measurements are parameters required in nuclear analytical techniques like neutron dosimetry and neutron activation analysis. They include:

- Average cross sections measured in well-characterised neutron fields like the ^{252}Cf spontaneous fission spectrum or reactor spectrum; examples of these are listed in the documentation of the IRDF-2002 dosimetry library [4], which are also available on-line from <http://www.nds.iaea.org/irdf/2002/html/>.
- Radiative capture resonance integrals and thermal cross section values [5], available on-line at <http://www.nds.iaea.org/reports/indc-nds-440.pdf>.
- Nuclear constants for neutron activation analysis [6] like Q_0 (ratio of the resonance integral and the thermal cross section) and k_0 (composite quantity involving gamma-ray emission probabilities and thermal cross sections of the measured nuclide and the standard, which is usually gold).
- Very low resolution cross-section measurements in lead slowing-down spectrometers [7], etc.

Basic nuclear data measurements address more directly the physical properties of the nuclei. They include decay constants and other parameters that characterise the emitted radiations from excited nuclei, cross sections for interaction of nuclei with incident particles of specific energies, angular and energy distributions of emitted particles, etc.

Data compilation, networks, databases and formats : The effort required on experimental measurements is enormous. By international collaboration (through regular scientific meetings between data producers and users, and through national, regional and international nuclear data committees) the task of data production is fairly well coordinated.

As produced, the results of experimental measurements and nuclear model calculations are scattered in various publications and hence inconvenient to access by a user. The need for a database, which would include all available experimentally measured basic nuclear data has long been realised. At present, there are four core Nuclear Data Centres, which regularly compile and update such a data:

- NNDC National Nuclear Data Center at Brookhaven National Laboratory serving USA and Canada (<http://www.nndc.bnl.gov/index.jsp>),
- CJD Nuclear Data Centre at Obninsk in Russia serving the former USSR countries (<http://www.ippe.obninsk.ru/>),
- NEA DB NEA Data Bank at Issy-Les-Moulineaux in France serving Europe and Japan (<http://www.nea.fr/html/dbdata/>),
- IAEA-NDS Nuclear Data Section of the International Atomic Energy Agency in Vienna, Austria, serving all other countries (<http://www.nds.iaea.org/>).

Together with a number of other smaller specialised nuclear data centres, they are organised into the Nuclear Reaction Data Centre Network (NRDC) to coordinate activities, share the work and exchange data so that the same up-to-date information in specific databases is available to all users, regardless of which data centre they contact. Additional organisational details can be found on <http://www.nds.iaea.org/nrdc.html>.

The International Network of Nuclear Structure and Decay Data Evaluators (NSDD) is organised and operated in a similar way. Additional organisational details can be found on <http://www.nds.iaea.org/nsdd.html>.

Due to the large amount of information, the databases must be managed in a computerized manner. Also, the formats for data storage must be well defined to allow automatic data maintenance and data retrieval. For this purpose, special formats for specific databases have been defined as follows:

CINDA compilation of bibliographic information related to neutron nuclear data. The database is available on-line from the main data centres, for example <http://www.nds.iaea.org/>.

NSR was originally intended to contain bibliographic information on the nuclear structure and decay data, but has been expanded to other types of nuclear data. The database is available on-line from the main data centres, for example <http://www.nndc.bnl.gov/index.jsp>.

EXFOR contains the actual experimental results in numerical form and other important information necessary for evaluation of experimental data. The strictly defined format [8] allows

easy exchange of data between all data centres. Like CINDA and NSR, the database is available on-line. CD-ROM Versions of the databases with the same user-friendly interface is available from the IAEA-NDS and can be ordered on-line from the IAEA-NDS web site <http://www-nds.iaea.org/>.

ENSDF contains nuclear structure and decay data and is maintained at NNDC. The data are available on-line from the main data centres as mentioned above. Other centres offer support like IAEA-NDS, which organises workshops for evaluators periodically. The information on workshops (when organised) is announced on the IAEA-NDS web site <http://www-nds.iaea.org/>.

The data centres also offer evaluated nuclear data libraries, processed files, application libraries and other information. The reader should consult the respective web sites.

Users assess the needs and express requests for new or more accurate data. In the past, such requests were compiled and published periodically by the IAEA in the World REquest list for Nuclear DAta (WRENDA) [9], but this publication is now obsolete. More recently the NEA Data Bank initiated a more systematic and rigorous approach to the compilation of a High Priority Request List maintained at <http://www.nea.fr/html/dbdata/projects/hprl.html>. In this way, laboratories that can perform experimental measurements have guidelines, which can help them to plan their activities so as to make their results directly useful to data users.

Nuclear model calculations : In recent years, a considerable improvement has been achieved in the capabilities of theoretical models [10] to predict cross-sections. Experimental data are preferred when available, but there are many cases where there are no experimental data (for example, for isotopes that are difficult to obtain in sufficient purity, rapidly decaying isotopes and data in energy ranges which make experiments more difficult and less reliable). In such cases, nuclear model calculations are used to interpolate or extrapolate experimental data, to resolve discrepancies between different experimental data, and to provide some data (although with greater uncertainty) for materials for which the experimental data are lacking altogether.

In computer program libraries like the Radiation Safety Information Computational Center RSICC at Oak Ridge (<http://www-rsicc.ornl.gov/rsicc.html>) or the NEA Data Bank in Paris (<http://www.nea.fr/html/dbprog/>), there are several nuclear model codes available. Many are specialised in specific reaction channels or energy ranges and very few address the problem of formatting the results in a form suitable for the exchange of nuclear data. Although they may be heavily used in the local

environments of a laboratory, they are not well suited for the evaluation work that is discussed in the next section.

Subgroup-A of WPEC (<http://www.nea.fr/html/science/wpec/index.html>) addresses the status and the development of the codes. From the working documents of the subgroup it is evident that the principal code systems suitable for general purpose evaluation work are the following:

- EMPIRE-II maintained by M. Herman (currently at NNDC, Brookhaven National Laboratory) and developed through international collaboration, with powerful graphics user interface for running the code and displaying the results interactively and data formatting capability. The package is available from IAEA-NDS on-line at <http://www-nds.iaea.or.at/> or on CD-ROM.
- TALYS developed by A. Koning [11], released recently and featuring integrated and robust coding, but without the data formatting interface. The code is available from the NEA Data Bank <http://www.nea.fr/html/dbprog/>.

Results of nuclear model calculations depend to a large extent on the input parameters. These input parameters for specific nuclides or a range of nuclides are available in the literature, but the information is scattered and the probability of typing errors or misinterpretation of the definitions is rather high. To improve the situation a project on the Reference Input Parameter Library (RIPL) was initiated at the IAEA-NDS, and contains tested sets of input parameters for nuclear model calculations. Interface modules had been developed for the EMPIRE-II and the TALYS codes. The database is available on-line at <http://www-nds.iaea.or.at/RIPL-2/> or on CD-ROM.

3.1.2 Nuclear data evaluation

All available data must be critically reviewed to eliminate or renormalize measurements that may be unreliable due to obsolete methods or systematic errors. It is the work of the evaluator to gather all available experimental information for a particular nuclide, make a critical review and decide on the “best estimate” value of the parameters. This is often done using sophisticated numerical procedures. When experimental data are abundant, one can use general least-squares technique to analyse the data statistically. Examples of such codes are:

- GMA Code System for Calculation of Reactor Accident Consequences [12]
- GLUCS A Generalized Least-Squares Code System for Updating Cross Section Evaluations with Correlated Data Sets [13]
- ZOTT ZOTT99 Generalized Least Squares Program [14]

The R-matrix least squares fitting codes have the advantage that they include additional physical

constraints based on theoretical models. This allows the use of additional measured parameters, which may be known with a better accuracy, but cannot be used directly. Examples of R-matrix codes are:

- EDA Energy Dependent Analysis Code for Nuclear Reactions [15]
- RAC R-Matrix code [16]
- SAMMY M6 : Code System for Multilevel R-Matrix Fits to Neutron and Charged-Particle Cross-Section Data Using Bayes' Equations [17]
- REFIT A Least Square Fitting Program for Resonance Analysis of Neutron Transmission and Capture Data [18]

The last two are specifically used for resonance parameter analysis. The disadvantage of the R-matrix approach is that the physics models are not exact and the propagation of model uncertainties is difficult to take into account. Evaluation of standard reaction cross sections for the ENDF/B-VI library was plagued by a small (but persistent) systematic discrepancy between general least squares analysis and R-matrix codes, and by unexplainably low uncertainties resulting from the R-matrix analysis. The problem was addressed through an IAEA CRP on the Improvement of the Standard Cross Sections and the participants believe that the problems are resolved. The report from the last research coordination meeting is available on-line on <http://www-nds.iaea.org/reports/indc-nds-463.pdf>, and preliminary evaluated cross section curves were released in December 2004. The full evaluated data set with uncertainties will become accessible at the end of 2005.

Evaluation of nuclear data in different energy regions requires different expertise, which is seldom available in a single laboratory. For example, in the USA the Oak Ridge National Laboratory contributes many evaluations of resonances parameters, while the Los Alamos

National Laboratory has the expertise to evaluate cross sections at higher energies. The results are then combined carefully to produce a complete evaluated data file. Another example is the international collaboration within the IAEA CRP to evaluate cross sections relevant for the thorium-uranium fuel cycle, which brings together leading experts from all major national projects. The objective is to reach consensus between all parties involved and produce evaluated data files that could then be adopted by national projects. The report from the second research coordination meeting is available on-line at <http://www-nds.iaea.org/reports/indc-nds-468.pdf>.

Evaluated data files are rather large and consist of highly-ordered data sets, grouped by materials and data types. They must be computer-readable, and in the past a number of formats evolved. One of the oldest is the British UKNDL format [19]. In Germany the KEDAK format [20] was designed. In the USA the ENDF series of formats were developed [21,22,23], version ENDF-6 being the most recent. The ENDF format (particularly ENDF-6) has received the most widespread acceptance: it has been adopted for the Japanese JENDL data library, the Chinese CENDL library, the Russian BROND library, the joint European JEFF files and also by the IAEA as the format for the exchange of nuclear data, thus making UKNDL and KEDAK formats obsolete. The ENDF-6 format specifications are continually improved to accommodate modern and complex nuclear data. Format proposals are discussed internationally by Subgroup B of WPEC and communicated to the Cross Section Evaluation Working Group (CSEWG) in the USA, which is formally responsible for the format and maintenance of the documentation. This format has also been adopted for the new ENDF/B-VII library in the USA, but alternatives that would take advantage of modern information technology are being discussed. This is a long-term commitment, since it requires careful

Table 1. List of evaluated data libraries

Country	Data file	format	Comments	Ref
Russia	BROND-2.2	ENDF-6	Available	[25]
China	CENDL-2	ENDF-5	Available	[26]
U S A	ENDF/B-IV	ENDF-4	(Old but useful for reference), available	[27]
	ENDF/B-V	ENDF-5	Restrictions on release lifted	[28]
	ENDF/B-VI	ENDF-6	Including Rev.8, 2001, available	[29]
	ENDF/B-VII	ENDF-7	Scheduled for release in 2005	
	JEFF-2.2	ENDF-6	Available	[30]
OECD/NEA	EFF-2.4	ENDF-6	European fusion file	[31]
	JEFF-3.0	ENDF-6	Available	[32]
	JEFF-3.1	ENDF-6	Scheduled for release in 2005	
	JENDL-3.2	ENDF-6	Available	[33]
Japan	JENDL-3.3	ENDF-6	Available	[34]

consideration to ensure unambiguous and clear data representation, as well as upgrading of all data processing codes. The full ENDF-6 formats manual is available on-line at <http://www.nndc.bnl.gov/nndcscr/documents/endl/endl102/endl102.pdf>.

Some of the more recent libraries, their formats and the country of origin are presented in Table 1. Most of them are available on-line from the IAEA-NDS at <http://www-nds.iaea.org/endl/index.html> or from the NNDC, Brookhaven at <http://www.nndc.bnl.gov/endl/index.html>. Many more libraries and special purpose files are available in the archives of the nuclear data centres [24]. The index is available on-line at <http://www-nds.iaea.org/reports/nds-7.pdf>.

3.1.3 Evaluated nuclear data processing

Basis for data reduction : Detailed information contained in the evaluated data files exceeds the capacity of the calculational tools (i.e. computer programs) for practical neutron transport applications. Some statistical Monte-Carlo programs can use such detailed information (reformatted for compatibility and better computational efficiency), but these codes require very fast machines. They are still mainly used for verification of results, difficult geometries, and to set up benchmarks.

Deterministic methods solve the differential or the integral forms of the transport or diffusion equation using one of the standard methods. They usually solve the one-neutron-speed form of the equation in the spatial domain (i.e. a one group equation), but the calculations are done for several groups albeit one at a time. The equations are coupled through the neutron transfer cross sections (scattering matrices) and the fission source. This means that the entire energy interval is divided into a number of subintervals known as groups. Within a group, each energy-dependent parameter takes some average value. The accuracy of the calculation depends on the number of groups and the group averaging method. Usually a compromise must be made between the complexity in geometry and the number of groups. The accuracy of the calculations can be retained even when the entire energy interval is divided into only a few groups, provided that a proper cross-section averaging method is implemented.

Data verification and validation : Automatic data processing is not possible unless the file is free of formal formatting errors. Next, the data in a file must be self-consistent. Before an evaluated data library can be used for practical applications, it must undergo thorough checking to avoid processing code failure due to format rule violation, to ensure that the data on the file correspond to what the evaluator intended them to be and that they are consistent with integral experimental measurements, when they are available. The following stages of data testing can be identified:

- removal of data formatting errors,

- removal of data inconsistency errors,
- visual inspection of the graphical representation of the data,
- comparison of the data on the file with the measured values (for example, from the EXFOR database),
- integral (spectrum-averaged) cross-section comparison with measured values,
- comparison with simple, clean experimental benchmarks (i.e. well-defined experimental set-ups that can be modelled with practically no assumptions or additional approximations).

Code packages available for data checking and verification include:

- ENDF Utility codes for checking data formats and internal consistency [35], developed at NNDC in Brookhaven and available on-line at <http://www.nndc.bnl.gov/nndcscr/endl/index.html>.
- ENDF Pre-Processing codes of the IAEA [36], available on-line at <http://www-nds.iaea.org/ndspub/endl/prepro/>
- ENDVER package [37] including user-friendly graphics user interface and integrating EXFOR retrieval, ENDF data reconstruction and powerful interactive graphics modules, developed at the IAEA-NDS and available on CD-ROM from <http://www-nds.iaea.org/>.

Data validation involves more sophisticated modelling of integral measurements and processing of evaluated nuclear data files into application libraries. Extensive programmes have been undertaken to validate the ENDF/B-IV and ENDF/B-V libraries. Reports on the testing of JENDL-3.2, JEF-2.2 and ENDF/B-VI have also been released, but the user must be aware of the diversity of data application. Suitable benchmark experiments are not always available and exhaustive data testing cannot be performed for all areas of interest. Compilations of benchmark experiments are already listed in Section 3.1.1.

Multigroup constants library generation : in updating or preparing a new multigroup constants library, the following pre-requisites are important:

- use a verified and validated evaluated data library,
- use validated processing codes.

The structure of any multigroup constants library is governed by the computer code used in conjunction with the library. The data processing procedures have to be considered on a case-by-case basis.

The choice of the data processing codes is rather limited. ENDF Pre-Processing codes [36] mentioned earlier were primarily designed for data verification, and lack modules like particle transfer matrix generation and applications library formatting. The most widely used code is the NJOY Nuclear Data Processing System [38],

which includes interface modules to many of the popular transport codes like the ACE library for the MCNP family of Monte Carlo codes, MATXS library format for deterministic transport codes, etc. An alternative is the AMPX system [39] developed at Oak Ridge. The strength of NJOY is its widespread use, which helped to identify and eliminate errors through international collaboration and highly efficient source code maintenance by the main author.

3.1.4. Nuclear data applications

The processed nuclear data are the basis for libraries for a large variety of applications. Some examples are listed below:

- small experimental thermal reactors,
- thermal power reactors,
- fast reactors,
- accelerator-driven systems
- nuclear fusion applications,
- shielding problems,
- radiotherapy,
- radioactive isotope production,
- inventory estimation, long-term storage etc.

Considering the different characteristics of the above-mentioned facilities and the sensitivity of cross section representation on the chosen group structure (illustrated in Figure 2) it is obvious that processed libraries must be strongly application-dependent. In calculations one normally starts from a selected multigroup constants library. Further data reduction is often performed by group condensation and spatial homogenization (Sections 3.3.4 and 3.3.5) to produce few-group parameters. Different types of data resulting from the processes described above are defined in the next Section.

3.2. Nuclear Data Types

The terms “nuclear data” or “cross section data” are applied to a wide range of specific data types appearing at different stages of data processing and reactor calculations. To avoid ambiguity it is useful to have precise definitions of these data types and the relation between them.

3.2.1 Basic nuclear data

Data resulting directly from experimental measurements or nuclear model calculations are implied. They include differential cross sections in energy and angle for neutrons and photons, resonance parameters and other data types that were already discussed in Section 3.

3.2.2 Evaluated nuclear data libraries

Evaluated nuclear data are constructed by an evaluation process (see Section 3.1.2) from the database

containing basic nuclear data. Evaluated nuclear data libraries consist of evaluated data files for individual isotopes, elements and/or compounds (at thermal energies, evaluations are made for the scattering properties of compounds where molecular and crystal lattice binding effects are significant). Databases of the basic nuclear data may contain several data points at a particular energy or may contain gaps where no data are given (subject to the availability of experimental data or nuclear model calculations). On the contrary, in an evaluated data file, a single parameter value must be prescribed at each point, with a precisely-defined interpolation law in-between points. The data must cover the full range of incident particle energies, usually from 10^{-5} eV to 20 MeV or higher. Recent trends in evaluated data files favour extension up to 200 MeV. Each parameter must be evaluated and checked for consistency with other parameters and integral measurements. The data are then entered on a file in a strictly defined format. Examples of evaluated data libraries were discussed in Section 3.1.2.

The energy dependence of cross sections is rather complex (some reactions may require more than 100 000 data points for accurate representation). Except for some Monte-Carlo programs that can read evaluated data in pointwise cross-section representation directly, data reduction techniques (i.e. group averaging) are needed.

3.2.3 Problem-Independent Group Constants Libraries

Problem-independent group constants libraries are derived from the evaluated data files. The parameters are averaged on a fine energy group structure, typically between 2000 and 200 groups (for example the SAND-II extended energy grid with 640 groups between 10^{-4} and 20×10^6 eV). A flat weighting function is usually sufficient. The group constants definitions are given in Section 3.3. So constructed libraries may be used as a source for group constants condensation into a coarser group structure (i.e. into multigroup constants) using some rough approximation to the problem-dependent neutron averaging spectrum as the weighting function. At this stage, the energy mesh is sufficiently fine so that local variations in the neutron spectrum can be disregarded.

3.2.4 Multigroup Constants Libraries

Multigroup constants libraries can be derived from the problem-independent group constants libraries by group condensation (see Section 3.3.4), or else they are calculated from the evaluated data libraries directly by using an appropriate weighting

function. The multigroup constants are broadly problem oriented, such as thermal reactors, fast reactors, fusion problems or shielding calculations. The criterion, which defines a group of problems for which a data set is

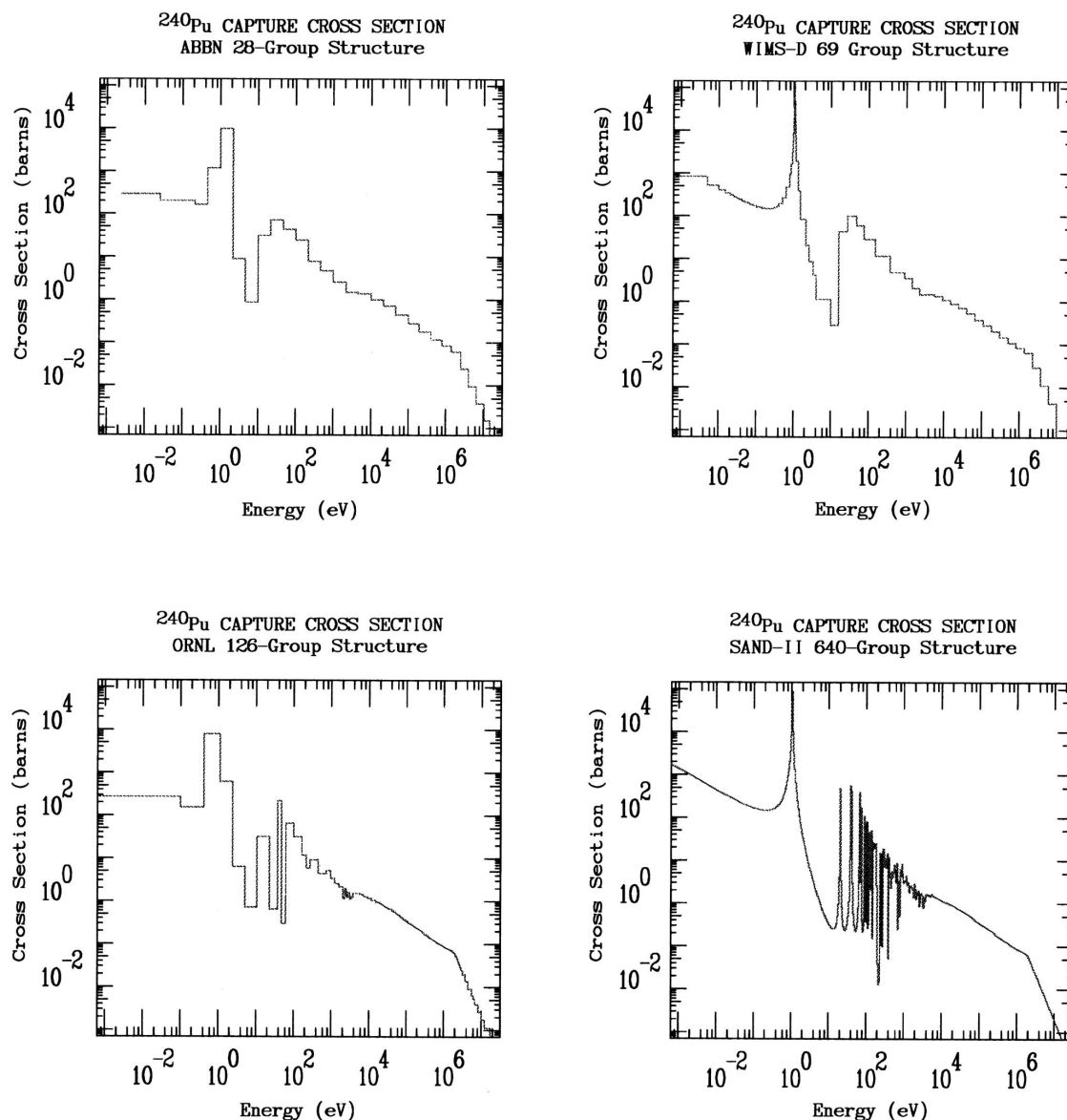


Fig. 2. ^{240}Pu radiative capture cross section from the ENDF/B-VI evaluated data library represented in various group structures.

valid, is the similarity in the smooth neutron spectrum (i.e. spectrum which exhibits the general characteristics but neglecting the detailed structure from resonances). Such a spectrum is used for weighting in the cross-section averaging process.

Consider for example an idealized infinite homogeneous reactor with hydrogenous moderator and a $1/v$ absorber at thermal energies (i.e. the absorption cross section is inversely proportional to the neutron velocity). The neutrons are born with the fission spectrum distribution. Assuming an idealized hydrogen-like medium with no absorption and a constant scattering cross section, the slowing down neutrons at epithermal energies have a $1/E$ distribution. With weak $1/v$ absorption at thermal energies, the resulting neutron spectrum has approximately a

Maxwellian distribution. A spectrum having a fission neutron spectrum shape in the fast energy range, a $1/E$ shape in the intermediate range and a Maxwellian shape in the thermal range is representative of thermal reactor problems over limited energy intervals, and is a candidate for the weighting function in the multigroup library preparation. Spatial variations of the neutron spectrum are not considered. For a desired accuracy in the calculations, the deviation of the local *true* neutron spectrum from the assumed one determines the required energy discretisation, which ranges typically from about 400 to 26 groups. Finer discretisation is required at energies where higher rates of reactions of interest are expected. Furthermore, inside each group, the smooth spectrum exhibits the general trend but not the detailed structure.

Allowance must be made for a detailed treatment, especially of the resonance self-shielding and Doppler broadening (usually in the form of separate tables). Interference between resonances of different nuclide constituents of a mixture is frequently neglected or treated very crudely.

To illustrate the cross section representation in group averaged form under different group structures, ^{240}Pu from the ENDF/B-VI evaluated data library [23] has been processed. The radiative capture cross section represented in four different group structures is shown in Figure 2.

For shielding problems where neutron spectra vary significantly with material composition it is not normally possible to obtain general multigroup libraries with fewer than about 50 groups (most of them being in the fast and epithermal energy region), whereas for reactor core calculations one can sometimes do with as few as 26 groups with emphasis in the thermal energy region.

3.2.5 Problem Dependent Few-Group Constants

Problem-dependent few-group constants are the result of the final stage of the data reduction process, starting from the multigroup data and using the neutron (and gamma) transport methods. The number of groups varies from 1 to 18 and spatial homogenization is also performed. Equivalent diffusion equation parameters (macroscopic cross sections and diffusion constants) can be deduced. Such data are highly problem oriented. They are calculated on a case-by-case basis and are normally considered as an application of nuclear data.

3.2.6 Example PWR Lattice

Light water reactor core neutronics design calculation is a convenient example, because it involves all stages of data processing and data types defined in the previous section. The calculational sequence is not unique, but for illustration the procedures of the CORD-2 package [40] are adopted, which uses the WIMS-D code [41] for lattice calculations. Figure 3 shows a typical 3×3 pin-array configuration, which is the minimum that can be considered in order to properly treat the leakage on the central pin boundary. The extra region on the outside is added to preserve fuel to moderator ratio of the overall assembly (including water holes, inter-assembly gaps and structural materials). The cross sections are calculated for the central cell only, which may contain a fuel pin, absorber rod or water channel.

Calculations start from the multigroup library. Preparation of the WIMS-D library within an IAEA-NDS coordinated research project is described in the documentation on the web site <http://www-nds.iaea.org/wimsd/>. Starting from the multigroup constants library, a zero dimensional (or approximate one-dimensional) calculation is performed (internally in the WIMS-D

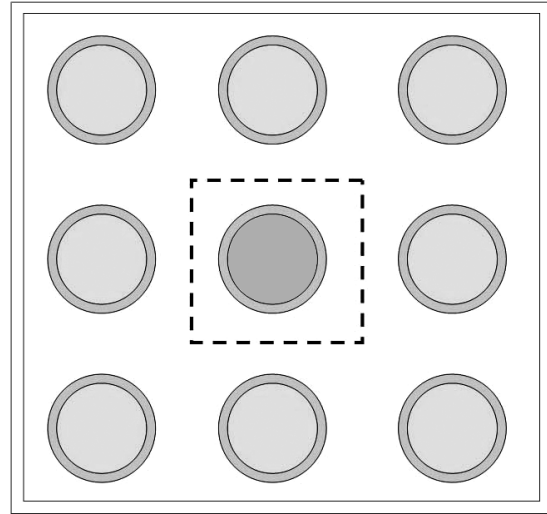


Fig. 3. Fuel pin array showing the central pin (bounded by dashed box), nearest-neighbour fuel pins and the extra region on the outside.

code), with appropriate material composition in individual homogeneous zones, to get an estimate of the local neutron spectra. These spectra are used to collapse the group constants (specific for each zone) down to typically 32 or 18 groups. In the WIMS-D family of codes this is the so-called spectrox calculation. With the reduced group structure, full-scale transport calculation for the pin array of Figure 3 is performed with a minimum loss of accuracy because the major features of the geometry and composition are explicitly considered in generating the spectra for group condensation. The results of the transport calculation are: central cell flux and neutron leakage values on the cell boundary, average flux values and few-group constants (usually from 1 to 12 groups) calculated by group collapsing and spatial homogenisation (using conventional flux and volume weighting to preserve reaction rates). This information can be used to further correct the few-group constants to preserve leakage [42], which is important for generating the constants for absorber cells. The few-group constants are macroscopic, i.e. they represent the average properties of the cell, including atom densities of the materials that constitute it. Whole-assembly calculations can be done with the few-group constants in the diffusion approximation. Applying the same group-condensation and spatial homogenisation principles with corrections for leakage over the fuel assembly, 2-group cross sections are defined that form the basis for coarse-mesh whole core calculations, which are typically needed in the reactor neutronics design calculations.

3.3 Definition of Group Averaged Constants

3.3.1 Single-valued energy dependent parameters

Conservation of reaction rates is the basic principle

for defining group-averaged values of simple energy dependent parameters such as cross sections, which are defined mathematically by the following equation:

$$\langle \sigma_x \rangle_g = \frac{\int_{E_{g+1}}^{E_g} \sigma_x(E) w(E) dE}{\int_{E_{g+1}}^{E_g} w(E) dE} \quad (1)$$

where: σ_x is the parameter to be averaged,
 w is the weighting function,
 E_g are the energy group boundaries,
 g is the group index.

The weighting function can be chosen arbitrarily, but from the aspect of reaction rate conservation when going from fine to broader group structures it can be easily seen, that the weighting function for averaging the cross sections must be the incident particle spectrum (i.e. the neutron or the gamma spectrum). Different weighting functions may be applied to other parameters, based on physical considerations.

For the construction of problem-independent group constants on a fine energy mesh, the weighting function is unimportant and can be assumed constant. In the case of the multigroup data, it is chosen as the smooth weighting spectrum which approximately follows the behaviour of the real spectrum. For thermal reactor applications it may consist of the Maxwellian form in the thermal energy range, the $1/E$ form in the epithermal energy range, and the fission spectrum in the fast range. Other applications (such as fusion or shielding problems) require a different weighting spectrum. Furthermore, each class of problems requires energy mesh refinement in different energy ranges, therefore it is not possible to construct a general purpose multigroup library which is reliable in all areas of application and have a reasonably small number of groups.

3.3.2 Differential energy-angle dependent parameters

The differential energy and angle scattering cross sections (elastic and inelastic cross section in the fast and the thermal energy range) can be group-averaged into the scattering matrix. The angular dependence can be taken into account through Legendre polynomial expansion. Elements of the l^{th} Legendre moment of the scattering matrix are defined by the following equation:

$$\langle \sigma_{s,l} \rangle_{g \rightarrow h} = \frac{\int_{-1}^1 d\mu \int_{E_{g+1}}^{E_g} dE w(E) \int_{E_{h+1}}^{E_h} dE' \sigma_s(E \rightarrow E', \mu) P_l(\mu)}{\int_{E_{g+1}}^{E_g} w(E) dE} \quad (2)$$

where : μ is the cosine of the scattering angle in the laboratory system,
 $P_l(\mu)$ Legendre polynomial of degree l
 $\sigma_s(E \rightarrow E', \mu)$ cross section for scattering from energy E into energy E' at an angle μ .

For elastic scattering and for inelastic scattering into discrete levels, the angle μ and the secondary particle energy E' are not independent. They are related through the laws of conservation of momentum and energy and defined by the mass ratio of the target nucleus to that of the secondary particle (for elastic scattering) and the reaction Q -value (for inelastic scattering into discrete energy levels). This considerably simplifies the technical process of producing scattering matrices. For inelastic scattering into the continuum and for inelastic scattering at thermal energies, additional data need to be processed (secondary neutron distributions and the scattering law data respectively). Alternatively, some approximations can be introduced, such as the “evaporation spectrum” to represent the secondary neutron distribution for inelastic scattering into the continuum and the “free gas” approximation for inelastic scattering at thermal energies.

3.3.3 Resonance region

The resonance integral is commonly defined by the equation:

$$RI = \int_{E_{g+1}}^{E_g} \sigma(E) w^*(E) dE \quad (3)$$

At infinite dilution (i.e. at small absorber concentrations which offer no perturbation to the neutron spectrum), the weighting function w^* is the usual smooth neutron weighting spectrum. In well moderated weakly absorbing systems, it has a $1/E$ form.

When a strong resonance absorber is present in an *infinite medium* with a high concentration, a significant fraction of the neutrons is absorbed and produces a “hole” in the neutron spectrum at the resonance energy, thus reducing the reaction rate. When an absorber of *finite dimensions* is surrounded by a moderator, the neutrons from the moderator tend to fill this hole. This is approximately analogous to the dilution of the absorber nuclei. However, this effect cannot propagate deeply into the absorber because the nuclei in the centre are shielded by the absorber nuclei on the surface, which remove the neutrons entering the absorbing medium at the resonance energy. Therefore the degree of the *effective* absorber dilution depends on the material composition and geometry.

Average cross sections of strong absorbers can be calculated by rigorously solving the slowing down equation for mixtures of the absorber with an idealized hydrogenous moderator of constant scattering cross section and different concentrations. In this way the self-

shielded absorber cross sections can be parameterised as a function of the Bondarenko background cross section σ_0 , which is the macroscopic “moderator” cross section per absorber atom (expressed in units of barns).

A rigorous solution of the neutron slowing down equation is rather tedious. Relatively simple approximations are available which produce satisfactory results, such as the Intermediate Resonance approximation (IR), introduced by Goldstein and Cohen [43]. A parameter λ is defined so that the cross section weighting function is:

$$w^*(E) = \frac{\sigma_0 + \lambda \sigma_p(E)}{\sigma_0 + \lambda \sigma_a(E) + \sigma_s(E)} w(E) \quad (4)$$

where : σ_0 is the Bondarenko background cross section,
 σ_a is the absorption cross section,
 σ_s is the scattering cross section,
 σ_p is the potential scattering cross section,
 λ is the Goldstein - Cohen parameter - a “measure” of the resonance width,
 $w(E)$ is the smooth spectrum (unperturbed by the resonances).

When $\lambda=1$ the well known Narrow Resonance (NR) approximation is obtained; when $\lambda=0$ the equation reduces to the Wide Resonance (WR) approximation. Goldstein and Cohen [43] used a variational technique to determine λ . Forti proposed a very simple approximation [44], which relates λ to the resonance width:

$$\lambda = \begin{cases} 1 - \frac{\Gamma_{p,r}}{2\alpha E_r} & ; \alpha > \frac{\Gamma_{p,r}}{E_r} \\ \frac{\alpha E_r}{2\Gamma_{p,r}} & ; \alpha \leq \frac{\Gamma_{p,r}}{E_r} \end{cases} \quad (5)$$

where : E_r is the energy of the r -th resonance,
 $\alpha = 1 - ((A-1)/(A+1))$
 A is the ratio of the mass of the target nucleus to that of the neutron,
 $\Gamma_{p,r}$ is the “practical width” [45] of resonance r , which measures the energy range over which the resonance contribution exceeds the nonresonance part of the cross section,
 $\Gamma_{p,r} = \Gamma_{tr} \sqrt{\frac{\Sigma_0}{\Sigma_p}}$
 Γ_{tr} is the total width of the resonance,
 Σ_0 is the macroscopic cross section at the resonance peak,
 Σ_p is the macroscopic potential scattering cross section of the absorber and the admixed moderator.

The above approximation is only applicable when addressing resonances individually. Alternative approaches to the definition of the λ parameter are based

on empirical derivations by matching the slowing down properties of an absorber diluted in an arbitrary medium and in idealised hydrogenous medium.

3.3.4 Group condensation

As mentioned in Section 3.2 the number of groups over which the cross sections are defined is often reduced by group condensation (or group collapsing). Assuming that the data are given on a fine energy grid, a weighting function is required that is averaged over the same energy grid. A number of fine groups can be collapsed into one coarse group by a procedure similar to the one defined by equations (1) to (3), except that the integral sign is replaced by a summation over the fine groups g , which constitute the coarse group h :

$$\langle \sigma_x \rangle_h = \frac{\sum_g \langle \sigma_x \rangle_g \langle w \rangle_g}{\sum_g \langle w \rangle_g}, \quad (6)$$

and similarly for the scattering matrices and the resonance integrals.

3.3.5 Spatial homogenization

Spatial homogenization can be performed using the same criterion of reaction rate conservation, using the spatial neutron flux distribution for weighting. Consider an energy group g and a homogenization volume V where r is the position vector inside V ; for clarity the group index is omitted. The average cross section is given by:

$$\langle \sigma_x \rangle = \frac{\int_V \sigma_x(\mathbf{r}) w(\mathbf{r}) dV}{\int_V w(\mathbf{r}) dV} \quad (7)$$

The scattering matrices and the resonance integrals can be averaged in a similar manner.

Such a simple flux and volume weighting procedure is valid when there is no leakage from the region, which is homogenized. In general, averaged cross sections homogenized by the simple flux and volume weighting satisfy the condition of average reaction rate conservation, but do not reproduce the partial neutron currents on the region boundaries. Recently, new homogenization methods have been developed [42], which to a large extent remove this deficiency and help to improve the results of global calculations.

4. STATUS AND TRENDS IN NUCLEAR DATA DEVELOPMENT

The computational power of modern computers and

advanced information technology methods allow efficient storing and handling of large datasets. Availability of graphics visualisation tools compensates partly for the difficulties of visual inspection of such complex data structures. General trends in the field of nuclear data can be summarised as follows:

- The bulk of the required data that can be measured easily is now available in the databases. Important contributions of new experimental measurements involve targets that are difficult to obtain or demand accuracies that require sophisticated experimental facilities. This is one of the reasons why so many small facilities have been shut down.
- Nuclear structure data help to improve nuclear models that are used extensively in nuclear data evaluation. They provide additional physical constraints, which improve the consistency of the data.
- Integrated graphics packages simplify the intercomparison of nuclear model calculations and experimental data, which helps in the optimisation of input parameters during an evaluation process.
- Significant progress has been made in developing methods that allow not only the estimation of “the best” values of evaluated parameters, but also their uncertainties and covariances.
- Systematic compilation of integral benchmarks and their analysis greatly increased the capabilities of benchmark testing of the data, which provides important feedback information to the evaluation process. At least for the area of conventional nuclear design applications, it is now possible to start from the basic evaluated data files, prepare application libraries from first principles, and predict the main integral parameters with an accuracy that was only possible before through tedious adjustments of the applications libraries.

New fields of nuclear data applications include:

- radioactive waste transmutation and innovative nuclear fuel cycle concepts,
- various analytical methods based on nuclear techniques,
- direct simulation of medical therapy or diagnostic techniques to improve the accuracy and reliability of the dose estimates to the patients,
- advanced techniques of medical radioisotope production of better purity, utilising specific features of the relevant reaction cross-section features,
- astrophysics.

New applications give rise to additional requirements for nuclear data:

- improvement of particle transport data above 2 MeV,
- extension of incident particle energies up to 200 MeV,
- evaluations for incident protons and other charged particles,

- inclusion of detailed photon production data,
- inclusion of covariance information at least for the most important nuclides and reactions.

Evaluated nuclear data libraries that are scheduled for release in the year 2005 will provide significant improvements in the quality and performance of the data, compared with the presently available libraries. These new databases will address some of the challenges posed by new applications, but a lot of the work remains to be done in the years to come.

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