Reference Input Parameter Library: Phase II (RIPL-2)

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Abstract

This report describes status of Reference Input Parameter Library (RIPL-2) being developed within the Co-ordinated Research Project carried out by the IAEA Nuclear Data Section. The library is 95% complete and its release is expected in July 2002.

INTRODUCTION

The Reference Input Parameter Library (RIPL) is a collection of input parameters for theoretical calculations of nuclear reaction cross sections. It is targeted at users of nuclear reaction codes and, in particular, at nuclear data evaluators. The first phase of the project completed in 1999, produced a Starter File and related documentation (TECDOC-1034). In 1999 the second phase of the project was initiated in order to test the RIPL-1 database and produce interfaces between RIPL and commonly used nuclear reaction codes. In course of work it turned out that substantial improvements and extensions of the original database are possible and worth of introducing. Therefore, the actual RIPL-2 database is considerably different from the original version.

The third Research Co-ordination Meeting of the RIPL-2 CRP was held at Vienna (Austria), 3 - 7 December 2001. The participants reviewed the status of work within the CRP. Library contents, testing, interfaces to the reaction model codes and retrieval tools were discussed. All files selected for RIPL-2 have been reformatted into the unified RIPL-2 format agreed during the second RIPL-2 meeting held at Varenna, Italy, in June 2000 (see INDC(NDS)-416). The participants also agreed on the uniform naming of the files in the RIPL-2 database. The actions and relative time-schedule were defined aiming in the completion of the RIPL-2 library be the end of February 2002 and its release in July 2002.

SEGMENT 1: MASSES

(co-ordinator S. Goriely)

The mass segment has been extended by inclusion of the file with abundances and Duflo-Zuker systematics and is considered to be almost complete. The masses based on the ETFSI model has been replaced with the more accurate data calculated in terms of the HF-BCS model. In addition, it was decided to include HFB matter densities which are necessary for calculation of optical model parameters within semi-microscopic approach (code MOM) in segment 4.

SEGMENT 2: LEVELS

(co-ordinator: T. Belgya)

The new version of the database has been submitted to the NDS. Compared to the RIPL-1 file the new database is updated and considerably extended. Several RIPL participants tested the preliminary version of the new database by using it in the calculations. A certain number of mistakes were found and most of the problems have already been corrected.

A simple test was worked out for checking nuclear temperature (T) derived from the analysis of cumulative plots of discrete levels. It yielded temperature values which are remarkably similar to the T(A) function obtained in the global fitting procedure. The performance of the T(A) function was tested by Ignatyuk by comparing it with the temperature obtained by Gilbert and Cameron. He has found reasonable agreement and recommended to use T(A) in cases for which no direct estimation is possible.

Herman tested N_{max} values (level scheme completeness) for nearly 500 nuclei using Gilbert-Cameron procedure and level densities specific to the EMPIRE code. A perfect fit was obtained for about 50% of analysed cases, fair agreement was found for about 25% and poor for the remaining 25%. It was noted that quality of the fit depends on the model used for level densities. No formatting errors were detected while reading files with discrete levels.

SEGMENT 3: RESONANCES

(co-ordinator: A. Ignatyuk)

The average resonance parameters of RIPL-1 were tested by the Brussels and Obninsk groups. Good agreement was found for Γ_γ among the tree RIPL-1 files (Obninsk, Mughabghab and Beijing). The comparison was less favourable for the neutron strength functions, especially for cases with large number of resonances.

It was concluded that additional data for neutron resonance spacings (D_{obs}), present in the Beijing file, are of uncertain origin (based on empirical systematics rather than experimental data) and should not be included in the RIPL-2 library. On the other hand, the revised average resonance parameters were obtained for 20 additional nuclei for which the data on resolved resonance parameters are available in the Sukhoruchkin compilation. This brings total number of D_{obs} in RIPL-2 to 301.

New evaluations of the average parameters for p-wave neutron resonances, prepared by the Obninsk group, should be included in the updated version of the RIPL-2 file as an additional column.

SEGMENT 4: OPTICAL

(co-ordinator: O. Bersillon)

The format of the optical model parameter (OMP) library was revised into the final form. The existing library was reformatted, and several corrections were made to the older potentials. Additions to the OMP library were made including new potentials from JENDL and from the Chinese Nuclear Data Center, as well as several new potentials from Bruyeres and Los Alamos. The new global potential for neutrons and protons from Koning and Delaroche was incorporated, as were new dispersive potentials from Capote. Kailas agreed to provide new optical potentials for α-particles, both as a limited selection of potentials for the OMP, and a subroutine for more general use. A file with deformation parameters for collective levels was provided by Fukahori.

An interface code (OM-RETRIEVE) was provided that will generate input files for SCAT2000 and ECIS96 from the OMP library. Utility codes for editing (OM-RIPLMOD) and summarising (OM-SUMRY, OM-TABLE) the OMP library were also provided. The OM-RETRIEVE code is to be revised to produce a concise table of parameters. Additionally, the OM-TABLE code will be changed to produce output tables ordered on Z and A of materials from the OMP library.

Where there are not enough experimental data to define phenomenological OM parameters one has to resort either to global parameterisations or to new microscopic approaches. The semi-microscopic model developed at Bruyeres is now part of the OM segment. This contribution consists of the MOM code which relies on the Jeukenne, Lejeune, and Mahaux nuclear matter approach, carefully revisited at Bruyeres.

SEGMENT 5: LEVEL DENSITIES

(co-ordinator: A. Ignatyuk)

Total level density

The updated versions of the recommended level-density files for the RIPL-2 were prepared but some final versions should still be submitted. There were the following additions and modifications:

-The revised version of the Back Shifted Fermi Gas (BSFG) model parameters consistent with both the recommended RIPL-2 neutron resonance parameters and the evaluated parameters of the recommended low-lying levels were prepared by the Obninsk group.

-The new BSFG systematics developed by the Brussels group, consistent with the recommended RIPL-2 neutron resonance parameters, were adopted for the RIPL-2 TECDOC.

-The Gilbert-Cameron (GC) and Generalised Superfluid Model (GSM) parameters were revised by Obninsk group in accordance with changes in the RIPL-2 resonance segment.

-The revised files for RIPL-2 were reformatted by R. Capote and included in the present version of the RIPL-2 library.

- -The microscopic HF-BCS calculations of the nuclear level densities supplied by Goriely were accepted for the RIPL-2 library.
- -The single-particle schemes used in the HF-BCS calculations were supplied by the Brussels group.
- -The FRDM single-particle schemes were reformatted by Capote and recommended as corresponding to the accepted FRDM mass table.

Partial level densities

Methods for calculating partial level densities for use in preequilibrium model calculations were critically reviewed. A microscopical formulation for the combinatorial calculation of particle-hole state densities based on a convolution of shell-model single particle-states with BCS pairing is recommended for inclusion in RIPL-2. Corresponding retrieval tools to obtain single-particle levels from Segment I tables were developed for RIPL2.

SEGMENT 6: GAMMA

(co-ordinator: M. Herman/V. Plujko)

The existing files in the Gamma segment were reformatted according to the RIPL-2 standard. The segment was enlarged by including the compilation of calculated GDR widths and energies provided by Goriely. Theory-supported practical approach, based on microcanonical description of initial states (modified Lorentzian (MLO)), for calculation of the dipole radiative strength function (RSF) was compared with the SLO end EGLO models. The subroutine, which calculates E1 γ-strength function for given A, Z, γ-ray and excitation energy, has been provided for the RIPL-2 library. The strength functions for other multipolarities will be carried over from RIPL-1.

SEGMENT: ANGULAR

The Angular segment will not be included in RIPL-2 library thus users interested in angular distributions in preequilibrium reactions will be referred to RIPL-1.

SEGMENT 7: FISSION

(co-ordinator S. Goriely)

Fission is a new RIPL-2 segment introduced during the last CRP meeting in Vienna. This segment will keep the RIPL-1 Maslov recommendation, but will include, in addition, global prescription for barriers and nuclear level densities at saddle points. In addition, a liquid drop estimate of the high-energy barriers will be provided.

RETRIEVAL TOOLS (WWW)

(co-ordinator: T. Fukahori)

The preliminary version of the RIPL-2 Home Page (http://wwwndc.tokai.jaeri.go.jp/~fukahori/RIPL-2/) and Top Pages for all segments have been prepared. Fukahori will continue to work on retrieval tools for particular segments.

TESTING

Testing has been performed for optical, resonance and levels segments. A number of misprints and erroneous coding has been detected and corrected. . Herman will check all FORTRAN codes.

The global testing of RIPL-2 database has been performed in three exercises. A large number of nuclear reaction cross sections was calculated with nuclear model codes EMPIRE-II, UNF and TALYS. Levels, optical model, and level density segments were verified and validated in these calculations.

Herman performed calculations for neutron induced reactions on 22 targets from ^{40}Ca up to ^{208}Pb in the energy range from 1 keV up to 20 MeV using EMPIRE-II code. There is a clear indication that calculations using new RIPL-2 files fit experimental data better than those with default EMPIRE-II parameters, which demonstrates improvement brought about by RIPL-2.

The second exercise has been carried out by the Beijing group. The calculations were performed for 103 nuclei from the mass region 69-160, in the incident energy range from 0.1 to 20 MeV, using recently developed code UNF. All input parameters were taken from the RIPL database. Agreement with the experimental data was found to be very good for total and elastic cross sections (within 3%). For other main reaction channels, calculations were able to reproduce the shape but some parameters' adjustments were necessary to fit absolute values of cross sections.

TALYS calculations were performed for various neutron-induced reactions on 5 isotopes from ^{52}Cr to ^{208}Pb. Default input parameters, originating from the RIPL-2 were used. This exercise concentrated on the comparison of Ignatyuk-type and microscopic level densities and provided reasonable agreement with experimental data for both formulations.

CODE INTERFACES

The work on interfaces between selected nuclear model codes and RIPL-2 segments has been continued facilitated by the standard RIPL-2 format. The two optical model codes (ECIS and SCAT2) and two statistical model codes (EMPIRE-II and UNF) use RIPL-2 library to a large extent. Interface code preparing inputs for ECIS and SCAT2 have been prepared by Young and is available in the optical segment. The UNF code makes use of RIPL optical potentials, masses, levels, level densities and GDR parameters. EMPIRE-II accesses RIPL-2 database directly and retrieves optical model parameters, discrete levels and microscopic level densities (HF-BCS). Built in systematics for GDR parameters and prescriptions for γ-strength functions follow RIPL-2 recommendations. EMPIRE-II library of masses and ground state deformations is numerically identical to the *mass-frdm.dat* in the mass segment of RIPL-2.

CONCLUSIONS

The RIPL-2 CRP is close to completion with most of the database collected at the NDS. Full drafts of the TECDOC chapters for mass, levels, optical, and gamma segments have been submitted. Partial drafts are available for level density and fission segments. In course of work the initial scope of the CRP was extended by including large amount of additional data and by replacing certain files with the updated ones. The release of the

RIPL-2 library is scheduled for July 2002.

At the end of the Vienna Meeting participants discussed possible improvements of the current project and formulated recommendations for further activities. These finding are summarised below:

-RIPL-2 library should be complemented with a set of routines for calculation of certain input parameters (such as level densities, binding energies, gamma strength functions, etc.) in order to facilitate user access to the database and to avoid misuse of the parameters.

-more attention should be dedicated to the use of microscopic models for producing parameters.

-parameters related to the fission channel contained in RIPL-2 need more accurate analysis and improvements.

-RIPL-2 provides good set of parameters for spherical and near-spherical nuclei. On the other hand, data for the deformed nuclei are scarcer and less accurate. In particular there is a need for Coupled Channels optical potentials and gamma-ray strength functions for the deformed nuclei. Also, the problem of collective enhancement of level densities should be addressed in more details in order to provide reliable prescription for calculating level densities in deformed nuclei. The latter are often needed for ADS and new reactor concepts.

-RIPL-2 concentrated on incident energies below 20 MeV, a typical limit for standard nuclear data files. However, new applications such as ADS or medical radioisotope production and radiation treatment need data at much higher energies (up to 1.5 GeV in case of ADS). Most of the parameters currently available from RIPL-2 can not be extrapolated to such high energies (e.g., temperature dependence of the GDR width). In particular, there should be consistency between statistical model calculations at low energies and the intranuclear cascade model commonly used at high energies.

-Special techniques should be applied for determination of the parameters for nuclei far from the stability line for which there are usually no experimental data available. These nuclei are important for ADS and astrophysics.

-Use of the results obtained in Heavy Ion induced reactions could be helpful in determining model parameters, especially for nuclei far from the stability line.

-Medical applications require charged particle reactions, which should be better represented in the parameter library.

-New experimental data from the recently initiated projects (HINDAS and NTOF at CERN) should become available within a year or two offering good possibility of testing RIPL-2 parameters.

The participants concord that these concerns should be addressed by a new CRP.