STATUS OF THE REFERENCE INPUT PARAMETER LIBRARY: PHASE II)

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April 2001

SUMMARY

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 1998, produced a Starter File and related documentation (TECDOC-1034). In 1999, the second phase was initiated in order to test the RIPL-1 data and produce interfaces between RIPL and commonly used nuclear reaction codes.
The second Research Coordination Meeting of the RIPL-2 CRP was held at Varenna (Italy) between 12 - 16 June 2000. The participants reviewed status of the work within the CRP. Library testing, interfaces to the reaction model codes, additions to the library and retrieval/presentation tools were discussed. In particular, issues related to level densities and shell corrections were debated in details. The participants agreed to undertake efforts in order to assure internal consistency and completeness of the library. Only those files, which fulfil these two conditions, will be accepted for the final version of the RIPL-2 library. In particular, this will lead to a substantial modification of the segments containing discrete levels and level density parameters. One of the major issues considered in details was the RIPL-2 format. The discussion resulted in the formulation and adoption of the homogenous RIPL-2 format for all the segments. The RIPL-1 recommended files that are accepted for the RIPL-2 will be converted into the new format. The same format will also be used for new submittals. The actions and relative time-schedule were agreed aiming in the completion of the RIPL-2 library by the end of 2001 and its release early in 2002.

In the following the status of work and recommendations in regard to RIPL-2 contents, format and testing are summarised.

SEGMENT 1: MASSES

(Coordinator: S. Goriely)

RIPL-2 will simplify and reformat (see Section 10) the data contained in Segment 1 of RIPL-1. Original files will be reworked in order to provide data of relevance without duplicating the same information. In particular, the audi.dat file will not be kept, the experimental masses being transferred to the FRDM and ETFSI files. The beijing.dat file does not contain data which are not already included in other files (masses are in FRDM, half-lives and spin in the Level segment, abundances will be provided in a separate file) and will consequently not be kept in RIPL-2. The jaeri-deformation.dat file will be kept but extended and moved to the Optical Segment. Segment 1 will be therefore reduced to:

- frdm95.dat file including experimental masses and FRDM predictions of masses, microscopic corrections and β deformations. The FRLDM and ε--deformations will not be kept,
- etfsi00.dat file including experimental masses and ETFSI-2 predictions of masses, shell corrections, β deformations and nuclear matter density distributions,
- expdef.dat file including the experimental β2 deformations of Raman et al. (1987),
- abundance.dat file with the terrestrial aboundances to be provided by A. Koning following

- dz.f Fortran code which will provide RIPL-2 with the systematics to be used if requested masses are missing in the frdm95.dat and etfsi00.dat files.

In addition, a clear definition of the shell and microscopic corrections will be added to the TECDOC. No other shell corrections, even if required in the Nuclear Level Density Segment (for example Myers & Swiatecki (1966)), will be given in Segment 1.

SEGMENT 2: LEVELS

(Coordinator: T.Belgya)

All files actually present in the Segment 2 of RIPL-1 will be removed and replaced by a new recommended file. The preliminary version of this file has been presented during the Meeting in Varenna. Contents of the file can be found in the format description later in this section. The file has been checked for multipolarity of γ-rays and for consistency of transition energies with γ-ray energies. In addition, sums of the decay branchings were checked. Additional checking by the CRP participants is in progress.

A new method of constant temperature fit has been used to determine cut-off energies for 641 nuclei that have more than 30 levels within a band of +- 4 mass units around the valley of stability. This procedure yields nuclear temperatures consistent with the values reported in the level density segment of RIPL-1 (bombay_gc.dat) except discrepancies around mass numbers 58 and 150 (for details see contribution by T. Belgya in Appendix 4). In addition, level density parameters *a*, extracted from the analysis of cumulative plots using Gilbert-Cameron matching condition were compared and proved consistent with those listed in the bombay_gc.dat file.

The formulae for calculation of transition probabilities for all decay modes will be provided.

The file containing results of fitting the cumulative plots will be reformatted according to the general RIPL-2 format specifications and will include T, U0, Nc, Nmax, Umin, and Uc. These data will be checked in co-operation with Ignatyuk and Capote with the GC formula using systematics.

Checking of the internal consistency of the Segment will continue and eventual problems in the ENSDF file will be reported to BNL evaluators.

SEGMENT 3: RESONANCES

(Coordinator: A. Ignatyuk)

The average resonance parameters of RIPL-1 were tested by the Brussels and Obninsk groups and the following points were noted:

- Chinese evaluation of D_o includes about 60 nuclei not available in the recommended Obninsk file. It is necessary to clarify the origin of these data and eventually to include them in the recommended file. The data for 34-S, 209-Pb and 142-Ce should be checked and , probably, corrected;

- New evaluations of the average parameters for p-wave neutron resonances prepared by the Obninsk group will be included into the RIPL-2 as an additional recommended file;
- The recommended file will be reformatted by the Obninsk group following general RIPL-2 format specifications.

SEGMENT 4: LEVEL DENSLTIES

(Coordinator: A. Ignatyuk)

Total Level Density

Contradictions between the average resonance spacings in the beijing.dat file and the average resonance spacings calculated with the Back Shifted Fermi Gas (BSFG) and Gilbert-Cameron (GC) models were noted by the Beijing group. General discussion of the recommended and others files included in this Segment indicates the need for a more complete definition of all model parameters used in the experimental data fitting. A necessity to supplement the recommended level density parameters with the corresponding systematics for all nuclei was confirmed by all the participants.

It was decided that RIPL-2 will include recommended (and only recommended) files for the three accepted models and microscopic level densities in the tabular form.

- For the Generalised Superfluid Model (GSM) the recommended reformatted file, together with the related systematics, will be prepared by the Obninsk group.
- For the BSFG and GC models, similar files will be prepared in collaboration by the Beijing and Obninsk groups. The contradictions of D_0 evaluated by these groups should be clarified and removed wherever possible. The level density parameter systematics will be provided for the BSFG and GC models. These will be supplemented with the detailed formulas or tables for the shell corrections, pairing parameters and other relevant quantities.
- Tables of microscopic nuclear level densities, based on HF+BCS single-particle schemes and including collective effects, will be provided by Goriely. Testing of these level densities has already been initiated (comparison with the average neutron resonance spacings).

Consistency checking of the recommended GC level density parameters with discrete levels in Segment 2 has been initiated and will continue (see also discussion of Segment 2).

Fission

The theoretical fission barriers will be supplied for all heavy nuclei by the Brussels group and will be included in the RIPL-2. The experimental fission barriers available in the RIPL-1 will be extended to lighter nuclei and reformatted in accordance with the accepted general RIPL-2 format specifications. The description of the level density for fission channels will be modified in collaboration with V. Maslov to reflect changes in the recommended experimental and theoretical fission barriers.

Partial level densities

The two methods for determining partial level densities (PLD) in pre-equilibrium model calculations were described in the RIPL-1 Handbook (TECDOC-1034). The first one consists

of closed formulae using the equidistant spacing model. The second is a semi-microscopic one, which employs single-particle level schemes contained in the RIPL-1 and relies upon combinatorial counting of the states. Limited testing of the both methods has been carried out. Good agreement between closed formulae and microscopic PLD was demonstrated for the deformed nuclei. However, large shell energy shifts that appear for near-magic nuclei can not be taken into account by any closed formula. In order to facilitate selection and use of PLD in nuclear model calculations recommended subroutines for PLD calculations will be extracted from the AVRIGEANU.FOR code. The microscopic PLD's for one, two and three particle-hole configurations can be calculated with the microscopic code already included in RIPL-1 using either Nix-Moeller or ETFSI single-particle level schemes. In RIPL-2 the latter two files will be split into elemental files. Appropriate interface code for reading these files and the updated code for the PLD calculations will be provided by Capote.

SEGMENT 5: OPTICAL

(Coordinator: O. Bersillon)

Many optical model parameter sets were collected for RIPL-1. Only those that cover a broad energy range are useful for production of nuclear data files since combining different sets results in the undesired discontinuities in cross sections. Therefore, it was decided to split the present selection into an archival part (containing essentially monoenergetic sets) and a users part, which will contain only global potentials. Moreover the most recent developments for neutron and proton o.m.p. at Bruyeres will be included in RIPL-2 after their release. This may require some extensions to the current format of Segment 5. The global o.m.p. for neutrons and protons on spherical nuclei as proposed by the Petten group will be introduced into RIPL-2 after its release In addition, 88 o.m.p. sets compiled in Beijing will be added. The RIPL-1 collection of o.m.p. will be extended by the compilation of o.m.p. for complex particles (up to α-particle) that will be provided by the Bombay group.
Where there are not enough experimental data to define precisely the o.m.p. one has to resort either to global phenomenological parameterisation or to new more microscopic approaches. . Such semi-microscopic approach developed at Bruyeres (revisited JLM) will be submitted to RIPL-2 starting with the case of spherical nuclei.
Coupled Channels and Distorted Wave Born Approximation calculations require the so-called experimental deformations for excited states. In order to satisfy this need it was decided to include in the RIPL-2 the compilation of experimental deformations published by Raman et al. in 1987. In addition, Fukahori will combine and submit to RIPL-2 experimental deformation used in various evaluation projects. For the purpose of identification, these files will reproduce discrete level record from the Segment 2.

SEGMENT 6: GAMMA

(Coordinator: M. Herman)

The RIPL-1 file *kopecky.dat* containing γ-strength functions has been reformatted by Plujko

RIPL-2 format specifications. Also, the Beijing file with GDR parameters will by reformatted to conform with the new specifications. These parameters will be supplemented with the shell dependent GDR widths derived form the ETFSI model and provided by Goriely. Additional systematics for M1 and E2 isovector Giant Multipole Resonances (GMR) will be provided by Fukahori. Obninsk group will supply new systematics for the parameters of E1, E2, and M1 GMR's.
The code *fE1_vs_A.for* for calculation of E1 γ-strength functions in the frame of the SLO, EGLO and TPA (Thermodynamic Pole Approximation) models has been provided by Plujko and will be included in RIPL-2.

SEGMENT 7: ANGULAR

(Coordinator: M. Herman)

No changes with respect to RIPL-1 are foreseen.

SYSTEMATICS

The role of systematics for nuclear model parameters was recognized by the participants of the Meeting. Actually, even relatively simple calculations on a stable isotope at moderate energies involve nuclei for which there are no experimental data allowing for the determination of the parameters. In such cases, one has to resort to systematics or approaches that are more microscopic. The RIPL-2 will attempt to address both possibilities. There are quantities which are difficult or impossible to systematise (such as masses, observed spacings of neutron resonances or shell corrections). For those (except D0) calculated numerical data will be provided in a tabular form for all nuclei between the two drip lines. For all others, appropriate systematics will be constructed. Each Segment in the TECDOC will contain at the very end a section with relevant systematics. In addition to the systematics already contained in the RIPL-1 following systematics will be included:

- energies of 2+ levels for the GSM.
- energies of 3- levels for the GSM.
- all level density parameters for GC, BSG, and GSM models. These will be compared with the recommended D0 values and cumulative plots of levels.
- Γ_γ from Gardner.
- Obninsk systematics for E1, E2, and M1 GMR parameters.
- Dufflo_Z subroutine for calculation of nuclear masses.

The quality of the systematics will be assessed by the plot of differences between systematics and experimental values (wherever available) in function of mass number. The resulting average standard deviation will serve as a global quality indicator. In the case of level densities, these will be supplemented by the comparison with the physical quantities as stated above.

RIPL-2 RETRIEVAL TOOLS

(Coordinator: T. Fukahori)

Web pages for retrieval of recommended masses, discrete levels (also in the GNASH format) and optical potential parameters based on RIPL-1 starter file have been prepared by Fukahori and made available at:.
http://wwwndc.tokai.jaeri.go.jp/RIPL/RIPL_mass.html and
http://wwwndc.tokai.jaeri.go.jp/RIPL/wripl/index.html
Retrieval of the optical model parameters is coupled with optical model code, which allows for on-line calculation of elastic angular distributions, total and absorption cross sections, S-matrix elements, and transmission coefficients. Plots of angular distributions, optical model potentials, and cumulative plots of discrete levels can be requested. These retrieval tools will be expanded so that the final Web interface will include (items within square brackets are tentative):

Masses:

- Audi, FRDM, ETFSI, and abundances (numerical data)

Levels:

- levels and decay data (numerical data and cumulative plots)
- Nmax (numerical data)

Resonance:

- D0 (numerical data)

Optical:

- index of optical potentials,
- cross sections: single energy, total, elastic, nonelastic, (numerical data)
- transmission coefficients (numerical data),
- S-matrix (numerical data)
- angular distributions (numerical data and plots)
- potential shape (plot)
- volume integral (plot)
- [total, elastic, and nonelastic cross sections in function of energy (numerical data and plots, comparison with TOTELA systematics above 20 MeV)]
- deformation parameters (numerical data)

Density:

Total and **Fission**:

- (numerical data, [plots including comparison with cumulative number of discrete levels and various level density formulae])
- microscopic (ETFSI) level densities (numerical data)
- D0 calculated using given model parameters and/or systematics (numerical data)

Partial:

- link to the codes

Gamma:

- GMR parameters according to Beijing and Goriely (numerical data)
- [GDR shape using different parameterisations (plot)]
- link to the codes.

Angular:

- link to the codes.

TESTING OF RIPL-1

Testing of the RIPL library concentrated mostly on the level density segment. Following tasks have been carried out by Capote:

- Software package for level density calculations within BSFG and GSM model were written and tested using RIPL-1 recommended parameters. Phenomenological level density code OBNINSK_BCS.FOR distributed with RIPL-1 was also tested.
- Microscopical code OBNINSK_MICRO.FOR, distributed with RIPL-1, was compared with microscopical Monte Carlo state density calculations using Nix-Moeller single particle levels.
- Phenomenological level density code OBNINSK_BCS.FOR, distributed with RIPL-1, was tested against Monte Carlo calculations mentioned above.
- Collective enhancement factors in the GSM formulation were compared with semi-microscopical calculation using Interacting Boson Model (IBM) for vibrational, rotational and transitional nuclei. The impact of negative parity states on the enhancement factor was evaluated for samarium and thorium isotopes.
- Microscopical particle-hole state densities calculated with the CAPOTE_MICRO.FOR code using Nix-Moeller single particle levels were compared with the results of AVRIGEANU's phenomenological code.

All microscopical codes in RIPL-1 proved to be complete. No strong dependence on the used single particle level scheme was observed in microscopical calculations. More work on the collective enhancement of the level densities is needed to improve currently used phenomenological recipes. It was shown that phenomenological closed formulae for particle-hole state density fails to describe microscopical calculation for magic nuclei. For deformed nuclei, like Sm-152, the agreement of Williams closed formulae using Kalbach pairing correction with microscopical calculations was very good.

In addition, a comprehensive testing of the level density parameters was performed by the Beijing group. The level densities were calculated for 303 nuclei using GC and BSG approaches and compared against experimental D0's and cumulative plots of discrete levels. Generally, better agreement was found for the GC approach but there is a clear need for improvement.

CODE INTERFACES

Progress has been made in preparing interfaces between RIPL and selected nuclear reaction codes. This work will continue being facilitated by the adopted common RIPL-2 format. Status of the interfaces is summarized below (note that most interfaces will need adjustments due to the new RIPL-2 format):

ECIS interface to prepare ECIS input from the RIPL library was coded by Young for the case of rotational nuclei. Further work is needed to include vibrational cases.

SCAT2 two interfaces were prepared independently by Young and Capote. Both

GNASH interface to GNASH optical model transmission coefficient file (tape10) for the RIPL-1 library has been completed with the optical model parameter retrieval code reported here. Similarly, implementation of a mass/spin-parity table (tape13) has also been implemented. Final interface will be based on the existing PREGNASH code after modification to the RIPL-2 format. Interface to the discrete levels (Segment 2) will be coded separately. RIPL-1 discrete levels in the GNASH format are already available on the WEB at: http://wwwndc.tokai.jaeri.go.jp/RIPL/wripl/index.html).
Development of the software package for the generalized superfluid level density model using RIPL parameters is under way (Ignatyuk and Young).

ALICE95 interface has been prepared by Fukahori but needs adjustment to the new format

SINCROS interface has been prepared by Fukahori but needs adjustment to the new format

EMPIRE-2 the code will access RIPL-2 library directly without any additional interface. Actually, EMPIRE-2.15.8 already makes use of data contained in RIPL-1 (optical model parameters, Ilijnov data for level densities, GDR systematics, and masses). Future releases will fully rely on RIPL-2 data (except EMPIRE specific level densities that will not be included in the official RIPL-2 version).

UNF the basic structure of the unified UNF code has been fixed and support for RIPL-2 will be developed.

STAPRE this code has been dropped from the list of supported codes due to lack of interest among the participants and to the fact that there is no reference version publicly available. It was also noted that the code is not capable of treating energies considerably higher than 20 MeV. However, in case appropriate interfaces are produced they will be included in RIPL-2.

TNG this code is not on list but in case appropriate interfaces are produced they will be included in RIPL-2.

CONCLUSIONS AND PERSPECTIVES

CRP participants agree that main emphasis should be given to internal consistency and reliability of the library. In particular, consistency between level densities, discrete levels and shell corrections must be assured. For each quantity, full information must be provided in order to avoid ambiguities in its use (e.g., level density parameters must be accompanied by relevant shell corrections used for their derivation). It was noted that providing computer codes for calculation of certain physical quantities from the RIPL-2 parameters might be beneficial to the users and would prevent misuse of the library. Standardization of the format will make RIPL-2 more users friendly and will facilitate preparation of interfaces to nuclear reaction codes. The new RIPL-2 library will contain fewer files compared to RIPL-1. As a rule only recommended, and well tested, files will be retained. On the other hand, RIPL-2 will be extended to comprise quantities that were missing or not adequately represented in RIPL-1 (such as aboundances and 'experimental' deformations). More attention will also be dedicated to various systematics with the ultimate goal to provide data for any nucleus between neutron and proton drip lines. A considerable amount of new data resulting from the ETFSI model will be included. These semi-microscopic data are particularly attractive

because of their internal consistency, wide range of nuclei, and quality comparable to the phenomenological ones. Considerable progress is expected in the optical model segment with the inclusion of new global parameterisations, semi-microscopic approaches and additional potentials for light complex particles. This new features should make RIPL-2 a unique and reliable tool for guiding theoretical calculations at incident energies up to 200 MeV needed for development of modern nuclear data.

The completion of the RIPL-2 library is scheduled for the end of 2001 and its release is expected in 2002. Recognising a crucial role played by the model parameters in nuclear data evaluation the IAEA Nuclear Data Section is planning to initiate a third phase of the RIPL project immediately afterwards. The principal goal of this phase will be to provide users with a set of tools for practical application of RIPL library in order to assure easy access to the data and proper use of the parameters.