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INDC International Nuclear Data Committee

Summary Report of Second Research Coordination Meeting

Parameters for Calculation of Nuclear Reactions of Relevance to Non-Energy Nuclear Application

(Reference Input Parameter Library: Phase III)

IAEA Headquarters, Vienna, Austria
28 November – 2 December 2005

Prepared by

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March 2006

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Abstract

A summary is given of the Second Research Coordination Meeting on Parameters for Calculation of Nuclear Reactions of Relevance to Non-Energy Nuclear Applications (Reference Input Parameter Library: Phase III), including a review of the various work undertaken by participants. The new RIPL-3 library should serve as input for theoretical calculations of nuclear reaction data at incident energies up to 200 MeV, as needed for energy and non-energy modern applications of nuclear data. Significant progress was achieved in defining the contents of the RIPL-3 library. Technical discussions and the resulting work plan of the Coordinated Research Programme are summarized, along with actions and deadlines. Participants' summary reports at the RCM are also included in this report.

March 2006

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SUMMARY

With recent formulations of nuclear reaction statistical models, nuclear reaction theory is believed to be in a position to meet many of the requirements for practical applications. The major sources of uncertainty are the input parameters needed to perform theoretical calculations. The IAEA has addressed these needs through a series of Co-ordinated Research Projects (CRP) on the Reference Input Parameter Library (RIPL), which involves the difficult task of collecting, evaluating and recommending the vast amounts of various nuclear parameters. RIPL is targeted at users of nuclear reaction codes and, in particular, at nuclear data evaluators. The first phase of the project was completed in 1999, with the production of a Starter File and related documentation (IAEA-TECDOC 1034)[1]. A second phase of the project was finished in 2002[2]. Substantial improvements and extensions to the Starter File have been made, resulting in a more accurate and reliable library. All files selected for RIPL-2 have been prepared in the unified RIPL-2 format, which facilitates their use in the reaction codes. The RIPL-2 library was released in July 2002 and is available on the web (http://www-nds.iaea.org/RIPL-2/). RIPL-2 constitutes a comprehensive and consistent set of nuclear reaction input parameters but its scope is limited to neutron-induced reactions up to 20 MeV, i.e., to a range typical for conventional power reactors. Addressing needs of other emerging nuclear technologies require extension of the RIPL-2 database to cover model parameters for calculation of nuclear reactions needed for non-energy applications such as: accelerator driven waste incineration, production of radioisotopes for therapy and diagnostics, charged particle beam therapy, and material analysis. In addition, there is a worldwide interest in nuclear astrophysics, which is constrained to rely on theoretical calculations of nuclear reaction cross sections to model distribution of isotopes in the Universe. To fulfill these requirements, the third and final phase of the RIPL project named "Parameters for calculation of nuclear reactions of relevance to non-energy nuclear applications" began in 2003.

The first Research Coordination Meeting (RCM) of the RIPL-3 CRP was held at IAEA Headquarters, Vienna (Austria) on 23-25 June 2004. A truly co-ordinated programme of work was agreed among the participants, leading to several additional actions to be undertaken. The participants agreed to undertake studies to ensure internal consistency and completeness of the library. Technical discussions and the resulting work plan of the Coordinated Research Programme were summarized in report published as document **INDC (NDS)-462**.

The second Research Coordination Meeting (RCM) of the RIPL-3 CRP was held at IAEA Headquarters, Vienna (Austria) from 28 November to 2 December 2005, and attended by ten CRP participants. The IAEA was represented by A.L. Nichols (Head, Nuclear Data Section), A. Trkov, A. Mengoni and R. Capote, who served as Scientific Secretary. M. Herman (BNL) was elected Chairman of the meeting. The approved Agenda is attached (Appendix 1) as well as a list of participants and their affiliations (Appendix 2).

The participants reviewed the status of the work within the CRP and discussed scientific and technical details. In particular, issues related to level schemes, level densities, optical model for deformed nuclei, fission barriers and parameter uncertainties were debated in detail. Summary reports of the work done by participants are attached (Appendix 3). The general structure of the RIPL database is well established and will remain unchanged. The expected output of the CRP will be an updated and expanded electronic database based on the RIPL-2 database, which will supersede the previous version. The first draft version of the chapters of the new RIPL-3 Handbook has to be sent by the Chapter's coordinator to IAEA by December 2006.

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[1] *Handbook for calculations of nuclear reaction data: Reference input parameter library* (International Atomic Energy Agency, Vienna, Austria, 1998), **IAEA-TECDOC-1034.**

[2] T. Belgya, O. Bersillon, R. Capote, T. Fukahori, G. Zhigang, S. Goriely, M. Herman, A.V. Ignatyuk, S. Kailas, A. Koning, P. Obložinsky, V. Plujko and P. Young. *Handbook for calculations of nuclear reaction data: Reference Input Parameter Library.* Available online at http://www-nds.iaea.org/RIPL-2/, IAEA, Vienna, 2005.

The main goals to be achieved within the new project remain those agreed during the First RCM (see **INDC(NDS)-462** report), in particular:

- Extend the library, including parameters needed for theoretical calculations up to 200 MeV for energy and non-energy applications.
- Establish well-defined and documented procedures for RIPL maintenance and future updates.
- RIPL validation using large-scale calculations of nuclear reaction across the periodic table (EMPIRE, TALYS, GNASH, UNF) and comparison with the available experimental database (including newest data from HINDAS, nTOF, etc.).
- Uncertainty estimation and/or range of parameter variation for RIPL.

The actions to be undertaken prior to the final RCM to be held at the end of 2007 were agreed; together with their relative time-schedule and deadlines (default deadline for all actions is the next RCM if not explicitly stated). The status of the work and the recommendations in regard to RIPL-3 contents, expansion of the library, validation and testing are summarized below:

SEGMENT 1: ATOMIC MASSES

Coordinator: S. Goriely

The following data will be delivered

- Skyrme HFB files including Audi *et al* (2003) evaluated masses. The HFB masses will be the most updated version in due time (S. Goriely; last update by end of CRP)
- FRDM (1995) including updated Audi *et al* (2003) evaluated masses (S. Goriely by June 2006)
- Skyrme HFB density distributions (corresponding to the nuclear masses provided) (S. Goriely; last update by the end of CRP)
- natural abundances as in RIPL2, but updated from Wallet Card 2005 (M. Herman by June 2006)

An investigation to include Gogny HFB nucleon densities will be undertaken, and if accepted the corresponding files will be prepared and sent to RIPL-3 (S. Hilaire by June 2006)

SEGMENT 2: DISCRETE LEVELS

Coordinator: R. Capote

The level scheme database was updated starting from the latest ENDSF update (October 2005) by T. Belgya under Contract Agreement with IAEA. The technical report describing the work done is included as Appendix 4. Newly derived discrete level (DL) files were distributed to participants for testing and validation. Format was not changed.

SEGMENT 3: RESONANCES

Coordinator: M. Herman

The discrepancies between new evaluation of neutron resonance parameters provided by S. Mughabghab with RIPL-2 evaluation were discussed. The following actions were agreed.

- review RIPL-2 and Mughabghab's Atlas predictions (June 2006, M. Herman)
- check discrepancies in ^{30}Si and ^{137}Xe (Christmas 2005, A. Ignatyuk)
- include new n-TOF measurements and send to M. Herman (R. Capote by June 2006)

SEGMENT 4: LEVEL DENSITIES

Coordinator: S. Hilaire

- Provide subroutine for shell correction energies and deformation energies (A. Ignatyuk by Christmas 2005)
- Provide code for K_{vibr} calculations, including updated compilation of 2+ and 3- collective states. (V. Plujko by March 2006)
- Provide total and p-h microscopic nuclear level densities (NLD) with normalization/interpolation subroutine (S. Goriely, S. Hilaire by Dec. 2006)
- Provide new tables of parameters and systematics for specified combinations of BSFG, GC and GS level density models (S. Hilaire, A. Koning by September 2006)
- Develop and test MODLIB module to estimate NLD using future RIPL-3 database (S. Hilaire, P. Talou by Christmas 2006)
- Provide ^{28}Si and ^{56}Fe (n,n') data from R.C.Haight (P. Talou)
- Provide stand-alone version of the Empire-specific NLD subroutine (M. Herman). Deadline: end of CRP.
- Provide systematic of LD parameters for EMPIRE specific level densities using RIPL 2/3 data (M. Herman). Deadline: end of CRP.
- Provide Monte Carlo computer code for microscopic single-particle LD calculations (R. Capote by Dec. 2006)

SEGMENT 5: OPTICAL MODEL

Coordinator: A. Koning

The participants agreed upon the following additional tasks and their relative deadlines (the default deadline is the next RCM if not explicitly stated):

- Investigate availability of global coupled-channel phenomenological as well as JLMB OMP (S. Hilaire, R. Capote by June 2006)
- Provide global deuteron OMP parameters (Y. Han by Jan. 2006)
- Provide LANL coupled-channel OMPs for nucleon induced reaction up to 150 MeV for selected fissile nuclei (P. Talou by Jan. 2006)
- Check, validate and interface double folding alpha potential provided by S. Goriely (R. Capote by June 2006)
- Provide regional alpha OMP in Fe region (M. Avrigeanu by June 2006)
- Validate the encapsulated OMP interface distributed at the Meeting (P. Talou by Dec. 2006)
- Update Web interface with ECIS and OPTMAN codes (T. Fukahori by Dec. 2006)
- Compilation of new OMP as provided by participants or retrieved from the literature (coordinated by Capote).
- Expand RIPL format as needed to accommodate new OMP potentials (Capote).
- Provide uncertainty or possible range of variation of the OMP parameters (Koning and Capote for phenomenological OMP, Hilaire for MOM). Uncertainties for KD03 global spherical OMP parameters were shown at the meeting by A. Koning. We should discuss how to put them into the database.

SEGMENT 6: GAMMA-RAY STRENGTH FUNCTIONS

Coordinator: V. Plujko

The participants agreed upon the following additional tasks and their relative deadlines:

- Provide an updated table with deformation parameters for GDR calculations (S. Goriely by Jan. 2006)
- Provide an updated table with experimental GDR parameters from IAEA Atlas (V. Plujko by Sept. 2006)
- Compare photo-absorption experimental data from Varlamov *et al.* with RIPL-2 recommendations (T. Fukahori).
- Provide updated file with experimental (Kopecky) radiative width based on RIPL-2 average spacing D0 (V. Plujko by Sept. 2006)
- Renormalization of the standard MLO1 gamma-strength parameters on both GDR data and low-energy experimental data. Provide new table of GDR parameters for MLO1 approach using photoabsorption data from the IAEA CRP (September 2006, Plujko).
- Test MLO1 gamma-ray strength function in hot nuclei (developed by Plujko for RIPL-3, see GAMMA segment) within EMPIRE system. (Herman)

SEGMENT 7: FISSION

Coordinator: S. Goriely

The participants agreed upon the following additional tasks and their relative deadlines:

- *Extensions of the RIPL-2 "experimental" barrier file* to include in addition to Maslov and Smirenkin barrier data, some recent analysis. These include about 20 nuclei analyzed in China (Y. Han), Am by Brookhaven (M. Herman), Th and Pa by the IAEA (R. Capote), U, Am and Pu by Los Alamos (P. Talou) and some more in Bruyeres (S. Hilaire). The new data should be sent by March, 2006 to R. Capote and should include the barrier heights, widths and symmetry, as well as the corresponding reference that should enable anyone to know the additional input parameters (in particular level densities, transition or class-II states, etc...) used in the data analysis. The name of the file should not include the "experimental" denomination.
- Investigate the possibility to include in RIPL-3 information on class-II states. The information will be centralized by P. Talou. S. Hilaire, Y. Han, R. Capote will send to P. Talou the data they have available. No information on transition states will be provided in RIPL-3
- Further development of the global HFB calculation of energy surfaces and the corresponding extraction of fission barriers heights and widths (S. Goriely, till the end of CRP)
- Further development of microscopic HFB plus combinatorial calculations of nuclear level densities at the saddle points (S. Goriely, S. Hilaire by Dec. 2006)
- Test and validation of the global microscopic inputs by S. Goriely, P. Talou, S. Hilaire, R. Capote, A. Koning on n-induced cross section by Dec. 2006
- Provide a code for calculating Madland-Nix fission neutron spectra. Get versions from Fukahori and Herman, and write one single code that will be tested and benchmarked against other codes and evaluations (P. Talou, till the end of CRP). Also, provide a suite of input parameters that have already been evaluated (like those used in recent IAEA evaluations)
- Work on GNASH calculations using Goriely's HFB predictions for the fission barriers and the level densities on top of saddle points (P. Talou, till the end of CRP).

RIPL-3 RETRIEVAL TOOLS

Coordinator: T. Fukahori

The detailed structure of the Webpage for retrieval of RIPL-3 database was discussed. It will be based on existing RIPL-2 web interface (http://www-nds.iaea.org/RIPL-2/). The RIPL-1 web-page is available at (http://www-nds.iaea.org/ripl/). 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. It was recommended to implement ECIS and OPTMAN codes within interface to be able to process all OMP parameters stored in the RIPL-3 library.

VALIDATION AND TESTING

The following actions were agreed:

- Perform large-scale nuclear data calculations throughout the periodic table using EMPIRE-II system to test the new RIPL-3 library (Herman). Deadline: End of CRP.
- Perform global test of the final RIPL-3 library with the nuclear model code TALYS by dripline to dripline calculations (Koning). Deadline: End of CRP.
- Provide comparison between Intranuclear Cascade (INC) and Hauser-Feshbach + preequilibrium calculations in high-energy nucleon induced reactions on selected actinides (Talou).

UNCERTAINTIES

- Provide a description of uncertainties affecting the data included in all the different RIPL3 segments, either in a well studied way or in term of general statements.
- All coordinators are responsible for providing in a way or another some information regarding the uncertainties affecting the data included in their segment.

Every segment of the future Handbook should contain information about corresponding uncertainties of the compiled data (Segment's coordinators).

UPLOADING AND DISTRIBUTING NEW FILES

The RIPL-3 temporal webpage has been set up on the NDS development server for distributing already available updated files (for example: new optical model interface and associated database). It is accessible by IP address (http://161.5.7.121/RIPL-3/).

The paswword-protected RIPL-3 web upload area has been set up on the NDS server running under Linux operating system for uploading new RIPL-3 files. Link will be added to the RIPL-3 temporal webpage. For the time being it is accessible as http://www-nds.iaea.org/ripl3_upload/

```
username: ripl3
password: reserved to the RIPL-3 participants
```

The directory structure is the same as the one of RIPL-2:

- ***masses***
- ***levels***
- ***resonances***
- ***optical***
- ***densities***
  - ***total***
  - ***fission***
  - ***partial***
- ***gamma***
- ***fission***

The files should be stored in the appropriate directories. The name of the file should start with the contributor's name followed by additional specification. For example, Plujko's file with GDR parameters should be named as *plujko_gdr.dat*
The directory name should not be repeated (masses, levels, etc.) in the filename. The general structure of the filename should be: [*author-]filename[_specification].dat* with items within square brackets being optional. Each file must be accompanied by the related file with description. These files should have *.readme* extension instead of *.dat* and should follow the RIPL-2 style. Related FORTRAN coding for reading the file is recommended for more complicated (non column-oriented) structure.

CONCLUSIONS

Presentations and discussions during the meeting showed very good progress of the work for the CRP. Actions agreed during First RCM were reviewed. Issues related to level densities, fission barriers and parameter uncertainties were extensively debated. A good agreement on the structure of the RIPL-3 level density segment was reached. A reasonable agreement on fission segment's contents was also reached, but will require further discussion in the light of the progress that will be made within the microscopic approach before the end of the CRP. An update of the RIPL-2 discrete level segment was carried out (see App.4). Further extensive work needs to be done in the next 24 months so that the necessary progress can be achieved before the final RCM. A truly co-ordinated programme of work was agreed among the participants, leading to several additional actions to be undertaken. The extension of the current project's timeframe up to 31 December 2007 was recommended by RCM participants', allowing for the last RCM meeting to happen at that time.

The general structure of the RIPL database is well established and will remain the same. The expected output of the CRP is going to be *an updated and expanded RIPL-3 electronic database* based on the RIPL-2 database. Minor format changes are expected to accommodate additional information needed for non-energy applications. The first draft version of the new RIPL-3 Handbook should be produced by December 2006.

The main goals to be achieved within the new project were clearly defined, including the maintenance and future update of the RIPL. Emphasis was placed on the determination of parameter uncertainties and validation using large-scale calculations of nuclear reactions across the periodic table. Complementary programming work on interface development was also recommended to make sure that observables predicted using RIPL-3 library have well defined and unique values.

The proposed features should make RIPL-3 a unique and reliable tool for guiding theoretical calculations at incident energies up to 200 MeV, as needed for modern energy and non-energy applications of nuclear data.

Second Research Co-ordination Meeting

"Parameters for Calculation of Nuclear Reactions

of Relevance to Non-energy Nuclear Applications" (RIPL-3)

IAEA Headquarters, Vienna, Austria

28 November – 2 December 2005

Meeting Room A0418

Monday 28 November

08:00 - 09:00	Registration (at Gate 1, IAEA Headquarters)
09:00 - 09:30	Opening session
	Welcoming address by IAEA/NAPC representative Election of chairman and rapporteur Discussion and adoption of the Agenda
09:30 - 10:15	**Coffee break, Administrative and Financial Matters**
10:15 - 12:15	Presentations and status reports (15' + 5' discussion each)
	S. Goriely S. Hilaire V. Plujko P. Talou M. Herman T. Fukahori
12:15 - 14:00	**LUNCH**
14:00 - 15:30	Presentations and status reports (cont'd), (15' + 5' discussion each)
	Y. Han E. Soukhovitski
	Invited report on validation: A. Ignatyuk
	Update of the Discrete Level and Optical Model Segments: R. Capote
15:30 - 15:45	**Coffee break**
	(From now on Chairman of the Segment is quoted in parenthesis)
15:45 - 18:00	Masses (S. Goriely), Levels (R. Capote) and Resonances (M. Herman).

Tuesday, 29 November

09:00 - 10:30	Gamma Strength Function segment (V. Plujko)
10:30 - 10:45	**Coffee break**
10:45 - 12:15	Interfaces and retrieval tools (T. Fukahori), Web
12:15 - 14:00	**LUNCH**
14:00 - 14:20	Presentations and status reports (cont'd), (15' + 5' discussion each) M. Avrigeanu
14:20 - 15:45	Optical model segment
15:45 - 16:00	**Coffee break**
16:00 - 17:30	Fission segment (S. Goriely)

Wednesday, 30 November

09:00 - 10:30	Fission segment (S. Goriely) (cont'd)
10:30 - 10:45	**Coffee break**
10:45 - 12:15	Fission segment (S. Goriely) (cont'd)
12:15 - 14:00	**LUNCH**
14:00 - 15:45	Fission segment (S. Goriely) (if needed) Level density segment (S. Hilaire)
15:45 - 16:00	**Coffee break**
16:00 - 18:00	Level density segment (S. Hilaire)
OPTIONAL:	*Dinner at Viennese Restaurant (not supported by IAEA)*

Thursday, 1 December

09:00 - 10:45	Level density segment (S. Hilaire) (cont'd)
10:30 - 10:45	**Coffee break**
10:45 - 12:15	Level density segment (S. Hilaire) (conclusions)
12:15 - 14:00	**LUNCH**
14:00 - 14:15	Presentation and status report: A. Koning
14:15 - 15:45	Optical model segment (A.Koning) (conclusions)
15:45 - 16:00	**Coffee break**
16:00 - 16:15	GANDR system for covariance estimation combining experimental and theoretical covariances (A. Trkov)
16:15 - 16:30	EMPIRE-KALMAN system: Uncertainty estimation of the input parameters using experimental data (M. Herman)
16:30 - 18:00	Uncertainty estimation of the RIPL parameters

Friday, 2 December

09:00 - 10:30	Discussion of the TECDOC layout (Assignment of tasks and deadlines for drafts)
10:30 - 10:45	**Coffee break**
10:45 - 12:15	Drafting the Meeting Report
12:15 - 14:00	**LUNCH**
14:00 - 17:00	Review and Approval of the Summary Report Closing of the Meeting

International Atomic Energy Agency

Second Research Co-ordination Meeting on

"Parameters for Calculation of Nuclear Reactions of Relevance to Non-energy Nuclear Applications"

IAEA Headquarters, Vienna, Austria

28 November to 02 December 2005

Meeting Room A0418

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Summary Reports by Participants

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IAEA Research Contract No. 12422
Progress Report on Research Project
"Microscopic optical potential for alpha-particles at low energies"

M. Avrigeanu[1], W. von Oertzen[2], F.L. Roman[1], and V. Avrigeanu[1]
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We show that the new experimental data reported by Galaviz *et al.* [Phys. Rev. **C71**, 065802 (2005)], for the α-particle elastic scattering on ^{112}Sn and ^{124}Sn at energies just below and above the Coulomb barrier, support the setting up of new physically meaningful local parameters of the optical potential, and the possible reconsideration of global potential parameter sets by using the existing data basis. The work carried out is being submitted to be published as the paper:
M. Avrigeanu and V. Avrigeanu,
Comment on "Elastic -scattering on ^{112}Sn and ^{124}Sn at astrophysically relevant energies"

Moreover, within the double folding formalism of the α -nucleus optical potential, used previously for a semi-microscopic analysis of the α-particle elastic scattering on A~100 nuclei at energies below 32 MeV, effects due to changes of the nuclear density at a finite temperature are considered. Parameterizations of the double-folding (DF) real potential as well as of a regional phenomenological potential have been used in the study of the (n,α) reaction cross sections for the target nuclei ^{92,95,98,100}Mo. Taking into account the microscopic DF potentials based on nuclear density distributions, we are able to fully describe the excitation functions of the (n,α) reactions. It is shown that the temperature dependence of the nuclear density distribution function can be an important aspect that has to be included in statistical model calculations even for a nuclear temperature smaller than 2 MeV.
The work carried out is accepted to be published as the paper:
M. Avrigeanu, W. von Oertzen, and V. Avrigeanu, *On temperature dependence of the optical potential for alpha-particles at low energies*, ***Nucl. Phys. A*** *(in press)*.

The same semi-microscopic analysis of the α-particle elastic scattering has been carried out also for the A~60 nuclei at energies below 49 MeV. The systematic of the corresponding OMP parameters is presently involved for setting a regional OMP parameter set also within this mass range. Finally, additional work is proposed in order to assist the further development of the RIPL-3 project.

IAEA Research Contract No. 13175
Progress Report on Research Project

Tokio Fukahori, Japan Atomic Energy Agency;
Nuclear Data Center, Tokai, Japan

Presentations and status reports

T. Fukahori reported the plan for www interface layout as a status report. Disscussed were which functions were needed for new RIPL-3 web pages. The results are summarized in next section.

Layout of the interfaces and retrieval tools and web

The RIPL-3 home page will include a summary description and link to the HANDBOOK

- The web page for "mass" segment contains same contents as RIPL-2 except to remove the information about ground state deformation. The abundance data will be replaced by those according to the new BNL wallet card (2005 version). The Q-value calculation tool will be also improved. The "Nuclear Matter Density" will be renamed as "Nucleon Density Distribution".
- Those of "levels" segment will be same as before, and the deformation parameters for excited levels will be moved from "optical" segment with the name of "deformation".
- Those of "resonances" segment will be same as before. It will be considered to replace RIPL-2 database with the new Mughabghab tables.
- Those of "optical" segment will be same as before, and the deformation parameters for excited levels will be moved to "optical" segment with the name of "deformation". The optical model calculation with ECIS and OPTMAN will be considered and double-folding calculation tool will be possibly provided.
- Those of "densities" segment will be same as before, and the programs used to plot will be checked. The 3-7 sets of combination of GC, BSFG, GSFM with/without enhancement factors will be given.
- Those of "gamma" segment will be same as before with adding MLO and theoretical GDR calculation.
- Those of "fission" segment will be same as before, and "Exp." will be renamed. New barrier evaluations will be added. Some additional information could be included, for example, fission transition states. The fission spectrum calculation tool (codes and inputs) will be considered to be added. The fundamental format will be kept as before. For new items such as deformed "nucleon density distribution", double-folding potential, evaluated fission barrier (extension into 3 or more) and fission spectra, the format must be considered.
- Interface for input data preparation for model codes (POD, COCOON, EMPIRE, GNASH, TALYS, …) will be expected to be produced as preparing parameters in "intermediate format" for "all" available channels with Q-value using CALAQ. Code developers can get information from this interface.

Actions

1) Interface and RIPL-3 web page discussed will be prepared based on RIPL-2 page.
2) One page introduction about web for TECDOC will be prepared.

IAEA Research Contract No. 12491
Progress Report on Research Project
"Parameters for Calculation of Nuclear Reactions of Relevance to Non-Energy Nuclear Applications"
(Reference Input Parameter Library: Phase III)

S. Goriely, Free University of Brussels; Faculty of Sciences;
Institute of Astronomy and Astrophysics, Brussels, Belgium

SEGMENT 1: MASSES

- New Skyrme HFB calculations were performed since the last RIPL-3 meeting. In addition to the already published HFB-03 to HFB-09 tables since the RIPL-2 publication, new improvements were performed recently. These are based on developing new effective interactions which also optimize the prediction of nuclear level density and fission observables. First results on mass predictions, as well as nuclear level densities and fission barriers based on the HFB-10 to HFB-12 models are presented to the RIPL-3 meeting.

SEGMENT 4: LEVEL DENSITIES

- A new global microscopic level density formula within the HFB plus combinatorial approach has been determined for the RIPL-3 project in collaboration with S. Hilaire. More details on the model can be found in the status report of S. Hilaire. These developments also include a new shell-dependent systematics of the quadrupole and octupole vibrational modes to estimate the vibrational enhancement factor of level densities

SEGMENT 5: OPTICAL

- A 900-lines code has been prepared to determine the three global double-folding alpha-potentials published in Demetriou et al. (2002, NPA707,253) for possible inclusion in the RIPL-3 library.

SEGMENT 6: GAMMA

- The original HFB+QRPA E1 strength as well as the folding code to determine the damping and deformation effects were sent to V. Plujko in October 2004, as agreed upon at the 2004 RIPL-3 meeting

SEGMENT 7: FISSION

- New fission barrier calculations were performed within the Skyrme HFB framework with an update effective interaction adjusted coherently on mass data (cf Segment 1)
- On Oct. 2004, the following data has been provided to P. Talou, A. Koning, R. Capote, M. Herman
  - full 1-dimensional shape barriers calculated within the HFB model
  - inverted parabola fits with barrier heights, widths and saddle point deformations
  - nuclear level densities calculated within the microscopic statistical model based on the single-particle levels at the saddle points deformation for n-induced fission on $^{235\text{-}238}$U, $^{238\text{-}242}$Pu, $^{241\text{-}243}$Am, ^{232}Th and $^{242\text{-}245}$Cm.

IAEA Research Contract No. 12842
Progress Report on Research Project

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Beijing; China

Measured reaction cross sections at 22.4 and 26.5 MeV and differential cross sections of elastic scattering for deuteron induced reactions on different nuclei missing from EXFOR library were obtained from figures and tables in published papers. The obtained data have been sent to IAEA/NDS on October 2004. The experimental data of differential cross sections of elastic scattering for ^{9}Be, ^{11}B, ^{12}C, ^{14}N, ^{16}O, ^{20}Ne, ^{24}Mg, ^{27}Al, ^{28}Si, ^{32}S, ^{40}Ar, ^{40}Ca, ^{48}Ti, ^{51}V, ^{52}Cr, ^{56}Fe, ^{59}Co, ^{58}Ni, ^{63}Cu, ^{64}Zn, ^{89}Y, ^{90}Zr, ^{93}Nb, ^{100}Mo, ^{103}Rh, ^{105}Pd, ^{107}Ag, ^{114}Cd, ^{115}In, ^{120}Sn, ^{140}Ce, ^{181}Ta, ^{195}Pt, ^{197}Au, ^{208}Pb, ^{209}Bi at different incident deuteron energy was considered in our analysis.

The program for automatically searching deuteron optimal optical potential parameters in the incident deuteron energy E_d<250 MeV has been developed. The input file and data of the code has been completed.
In order to validate the obtained RIPL, UNF and MEND codes were used to calculate neutron and proton-induced reactions and compared with the available experimental database for some nuclei.

ENERGY DEPENDENCE OF THE OPTICAL MODEL POTENTIAL

The real part of optical potential

$$V=V_0+V_1E+V_2E^2+V_3(N-Z)/A+V_4Z/A^{1/3}.$$

The imaginary part of the surface absorption

$$W_s= W_0+W_1E+W_2(N-Z)/A.$$

The imaginary part of the volume absorption

$$W_v= U_0+U_1E+U_2E^2+U_3(N-Z)/A.$$

The spin-orbit potential

$$V_{so}=V_{so1}+iW_{so}$$

OMP PARAMETERS

V_0=82.17832, V_1=-0.14809, V_2=-0.00088571, V_3=-34.81102, V_4=1.05844,

a_r=0.80924, r_r=1.17363

W_0=20.96773, W_1=-0.079392, W_2=-43.39772

a_s=0.46490+0.045$A^{1/3}$, r_s=1.32752

U_0=-4.91585, U_1=0.055454, U_2=0.00004417, U_3=35.0,

a_v=0.70000+0.045$A^{1/3}$, r_v=1.56287

V_{so}=3.70233, W_{so}=-0.20589, a_{so}=0.81300, r_{so}=1.23351.

r_c=1.69773

IAEA Research Contract No. 12843
Progress Report on Research Project

Michal Herman, Brookhaven National Laboratory;
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RIPL-2 database was extensively used in the evaluations being prepared for the ENDF/B-VII library. As many as 69 totally new evaluations were prepared using EMPIRE-II system with RIPL-2 library using as default for all model parameters. Taking into account that about 25 nuclei are being involved in a single evaluations, and that there is a natural overlap of nuclides when an isotope chain is evaluated the total number of nuclides tested in these calculations was about 1000. It should be stressed that evaluation procedure implies more thorough level of testing than blind calculations across periodic table. In general, modification of the default parameters was necessary in order to reproduce experimental data but the initial values were quite good starting points and they were kept for the cases where no experimental cross sections were available. No critical errors (causing fatal error in the EMPIRE code) were encountered. The only annoying feature was discrete levels with undefined energy (+X) that caused problems in the ENDF-6 format and were distorting calculations. This problem has already been solved in the RIPL-3 database.

A new evaluation of neutron resonances and associated quantities has been completed by Said Mughabghab. This analysis is a continuation of the well known BNL-325 compilation, of which the last edition was published in 1984, and takes into account all experimental data on neutron resonances published until 2005. Of interest to RIPL-3 will be average quantities such as neutron spacings for s- and p-waves and gamma widths. The initial comparison of neutron spacings shows that in a number of cases there are significant differences between RIPL-2 database and the new evaluation. The agreement is much better for the gamma widths. The new Atlas of neutron resonances has been submitted for publication and is expected to be available by March/April 2006. Once the data are public RIPL-3 should review discrepant cases and eventually update the current resonance segment.

The FORTRAN module used to calculated EMPIRE-specific level densities has been extracted from the EMPIRE system and made into a stand-alone code. The EMPIRE-specific approach offers a number of advantages compared to the classic Gilbert-Cameron or Back-Shifted Fermi Gas models still preserving computational convenience of the closed-form approximation. Work is in progress on adding minimization routine in order to re-parameterize EMPIRE-specific level densities using RIPL-3 recommended data including neutron resonance spacing, shell corrections and RIPL-3 methods. In particularly, a method to estimate the vibrational enhancement factor selected by the RIPL-3 participants along with table/systematics of vibrational states will be used in fitting. In addition, deviations from the rigid-body moments of inertia might be considered. The resulting level density parameters and associated systematics will be determined and provided along with the EMPIRE-specific level density FORTRAN module.

IAEA Research Contract No. 13068
Progress Report on Research Project
"Work performed on microscopic level densities using the HFB + combinatorial method"

S. Hilaire, CEA/DAM, Ile de France;
Centre d'etudes nucléaires de Bruyères le Châtel (CEN);
Service de physique nucléare, Bruyères le Châtel, France

S. Goriely, Free University of Brussels; Faculty of Sciences;
Institute of Astronomy and Astrophysics, Brussels, Belgium

A new Skyrme force has been developed in order to fit experimental masses with a pairing strength constrained on the odd-even mass differences. Using the HFB method with this force, single particle level schemes for both protons and neutrons have been generated for nearly 8000 nuclei. The combinatorial method has been applied to compute for each nucleus both the particle-hole and total state densities as a function of the energy, spin projections and parities.

Rotational bands are explicitly treated to go from state densities to level densities, and the transition from deformed to spherical shape is also accounted for. Vibrational modes are treated using a phenomenological expression determined to fit the available experimental data for quadrupole and octupole phonons' energies. This new phenomenological expression includes shell effect to deal with the structures observed when looking at these experimental energies.

The currently obtained results give an average accuracy comparable to what can be obtained with a global Back Shifted Fermi Gas model or to that already available with the HFB + statistical level densities of RIPL II. The impact of these new tabulated HFB + combinatorial level densities has also been studied with the TALYS code and tested on different cases.

IAEA Research Contract No. 12891
Progress Report on Research Project

A. Koning, Nuclear Research and Consultancy Group; Fuels, Actinides and Isotopes,
Petten , Netherlands

Uncertainties of the KD03 global optical model parameters

An estimate of the uncertainties of the parameters of the KD03 global optical model potential has been given. A Monte Carlo method for generating uncertainties of the final cross sections and angular distributions is used. The approach is pragmatic: The parameter uncertainties are adjusted such that the resulting calculated uncertainties account for the difference between the global prediction and the experimental data. At this stage, no OMP parameter correlations have been taken into account. We think however that the present results, summarized in the Table below, allow for adjustment of OMP parameters for data evaluation purposes. The presented uncertainties give a measure of the allowed deviation from the average parameters.

r_v	2	D1	10
a_v	2	D2	10
V_1	2	D3	10
V_2	3	r_{so}	10
V_3	3	a_{so}	10
V_4	5	V_{so1}	5
W_1	10	V_{so2}	10
W_2	10	W_{so1}	20
r_D	3	W_{so2}	20
a_D	4		

Table 1. Uncertainties of the global neutron OMP parameters, given as fraction (%) of the absolute value.

Phenomenological level density parameters

A computational set up for a consistent parameterization of three level density models has been built. This includes the Back-shifted Fermi gas Model, the Constant Temperature Model and the Generalized Superfluid Model, each without and with explicit collective enhancement. The resulting level densities should be applicable over a large energy range, taking into account experimental information from both discrete levels and mean resonance spacing. For each of the three models, we have produced local level density parameters, i.e. parameters that are adjusted per nucleus, which give the best average description of all observables (discrete levels, mean resonance spacing) for that nucleus. We have also produced a global level density parameterization for all models, i.e. formulae for the global expressions that enter the level density formula, to be used for any nucleus. A few remaining deficiencies in the procedure need to be removed before the parameter collection can be delivered to RIPL-3.

IAEA Research Contract No. 12492
Progress Report on Research Project

"Improvement and testing practical expressions for E1 strength functions and vibrational enhancement of nuclear level densities within semiclassical approach"

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Physical Faculty; Nuclear Physics Deparment, Kiev; Ukraine

Numerical studies performed during period under report indicate that the calculations of the radiative strength functions within the closed-form models give similar results in a range of gamma-ray energies around the GDR peak.

However the results within MLO and EGLO models are different from SLO model calculations in the low energy region. In particular, for E_γ =7 MeV, the calculated RSF values within SLO model are about two times greater comparing to the ones obtained for MLO and EGLO models (excluding the atomic mass range $A \in$ 150-180 for EGLO model).

There is a substantial distinction for some nuclei between the calculation results obtained in microscopic QRPA(RIPL2) model and semiphenomenological MLO approach and experimental data, but for QRPA(RIPL3) this discrepancy is smaller. It should be stressed that the RSF within closed-form approaches are in a rather good agreement with experimental data for gamma-ray energies near GDR peak. Note that in contrast to closed-form methods, all deformed nuclei are considered to be prolate ones in the QRPA.

The overall comparison of the calculations within different models and experimental data showed that MLO and GFL provide the most reliable simple methods for determining the E1 radiative strength functions over a relatively wide energy interval ranging from zero to above the GDR peak. The MLO and GFL are not time consuming calculational routes and can be recommended for general use; both of them can be used to predict the photo-absorption cross-sections and to extract the GDR parameters from the experimental data for nuclei of middle and heavy weights.

It should be noted that a collisional component of the GFL damping width can become negative in some deformed nuclei.

It seems that the semi-microscopic model with moving surface (MSA) and microscopic QRPA(RIPL3) are more adequate for estimation of the RSF in spherical nuclei if reliable values of the GDR parameters are not available.

Response function (RF) method was also considered and tested to describe the effect of the vibrational states on nuclear level density. The method allows to take into account the damping of vibrational states in a standard semi classical way.

The calculation of the vibrational $2^+ \otimes 3^-$ enhancement factor (K) within the RF method and different phenomenological approaches were compared. Calculations within the RF approach agree better with that ones within the methods of boson partition function with average occupation numbers (BAN) and boson partition function with damped occupation numbers (DN). They are also in rather close agreement with the results of a finite temperature extension of IBM.

The calculations demonstrate rather strong dependence of the vibrational enhancement factor K on vibrational state damping. Using boson partition function with average occupation numbers (BAN) is the best method to calculate the vibrational enhancement factor when N/Z dependence of asymptotic level density parameter is taken into account.

$$\tilde{a} = (0.1286A - 0.04872A^{2/3}) / \exp(0.0002986(N-Z)^2)$$

Method of boson partition function with damping occupation numbers (DN) is the best one without allowance for N/Z dependence of asymptotic level density parameter

$$\tilde{a} = 0.103A - 0.105A^{2/3} \quad (RIPL2)$$

IAEA Research Contract No. 13067
Progress Report on Research Project

"Coupled-channels optical model potentials for calculations with coupling built on soft-rotator model for nucleon induced reactions up to 200 MeV incident energies in A =24-120 mass region"

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Nuclear Data Laboratory, Minsk, Belarus

During these nine months the Research Contract activity was developing according to the schedule as fixed in the Contract.

Developing a global optical potential for even-even nuclides with A = 24-120 mass for coupled-channels optical model calculations based on coupling built on soft-rotator nuclear model Hamiltonian wave functions we already:

1. Determined Nuclear Hamiltonian parameters describing low-lying collective levels of even-even nuclides with A = 24-120 mass for all nuclides having experimental optical data available.
2. Formatted all the available optical experimental data for even-even nuclides with A = 24-120 mass into input of OPTMAN code for optical potential search option. Data still unavailable in the EXFOR database was submitted to the Nuclear Data Section for inclusion.
3. Derived a local OMP parameters for even-even A = 24-120 mass nuclides.
4. Release the OPTMAN code's user guide with the support of our Japanese collaborators. The User guide was published as JAERI technical report as cited below:

E.Sh. Soukhovitskiĭ, S. Chiba, O. Iwamoto, K. Shibata, T. Fukahori, G.B. Morogovskij (JAERI technical report "*Programs OPTMAN and SHEMMAN Version 8 (2004)"*, JAERI/Data-Code 2005-002, 2005). It is freely available on request from Japanese Nuclear Data Center.

Global optical potential for even-even nuclides with A=24-120 mass, which is the main goal of the Contract's first year activity, will be derived based on individual optical potential parameters already determined.

This research contract made possible very fruitful international scientific cooperation aimed to incorporate ideas on dispersive relationships between imaginary and real parts of optical potential developed earlier by Roberto Capote (IAEA/NDS) and Jose Manuel Quesada (Seville University) in the CC optical code OPTMAN. The real possibility to use a modified OPTMAN code for high priority practical applications arises. These activities are coordinated through RIPL CRP. We determined an excellent optical potential for ^{232}Th nucleus, allowing to describe all the available optical experimental data from 1 keV to 200 MeV within 1.5 experimental errors in average. This potential was recommended to be used in IAEA ^{232}Th evaluation and was already included in RIPL library. This is a significant result of international cooperation of scientists from Belarus, IAEA, Japan and Spain, that became possible due to the Contract and is beyond the Contract working plan. The work was already published at *Physical Review **C72** (2005) 024604***,*** (E.Sh. Soukhovitskii, R. Capote, J.M. Quesada and S. Chiba, *Dispersive coupled channel analysis of nucleon scattering from ^{232}Th up to 200 MeV*)

Preliminary investigations proved that we can get derive very good CC optical potential for actinides based on new dispersive ideas incorporated in OPTMAN code. The same is true for structure materials. So we added corresponding tasks to the second year of the Contract.

IAEA Research Agreement No. 12795
Progress Report on Research Project

P. Talou, University of California; Los Alamos National Laboratory (LANL);
Theoretical Division; Group T-16, New Mexico, USA

We have proposed new coupled-channels optical model potentials to be included in the RIPL database. These potentials concern nucleon-induced reactions up to 150 MeV for selected fissile nuclei. They will be sent to the CRP secretary by March 2006.

Intra-nuclear cascade calculations were carried out using the CEM2k code in order to calculate prompt fission neutrons spectra from 20 to 150 MeV. These calculations have been shown to perform very well for selected nuclei and energies below 150 MeV, where the use of INC calculations is questionable. Those results can provide useful benchmarks for extending fission neutrons spectra calculations above 20 MeV.

A study of the ^{89}Y(n,2n) reaction covariance matrix was presented, demonstrating significant, but understandable, differences in covariance matrices evaluated from experiment or from model calculations alone. The KALMAN code was used for that.

Finally, GNASH calculations of the (n,f) and (n,2n) cross sections for some actinides were performed, using Goriely's HFB calculated fission barrier parameters and nuclear level densities at saddle points. More work remains to be done on this item, in order for the outcome to be of any use for the present project.

At our last meeting, several actions were also decided for LANL to carry out during the coming year. Here is the list of these actions:

- Provide ^{28}Si and ^{56}Fe (n,n') data from R.C.Haight;
- Send optical model potentials used at LANL for several isotopes, as described in our last progress report;
- Provide experimental information (if any) on class-II states;
- Provide a code for calculating Madland-Nix fission neutron spectra. Get versions from Fukahori and Herman, and write one single code that will be tested and benchmarked against other codes and evaluations. Also, provide a suite of input parameters that have already been evaluated (e.g., get input parameters from Ignatyuk as obtained in the Thorium CRP);
- Provide a MODLIB module to calculate level densities within the GSF, GC, and BSFG models. Get pieces of codes from Hilaire;
- Work on GNASH calculations using Goriely's HFB predictions for the fission barriers and the level densities on top of saddle points.

RIPL-X discrete levels

T. Belgya

Summary

The RIPL-2 discrete level library was created during the RIPL-2 CRP period of 1998-2002 from an ENSDF data set that was used to update the Table of Isotopes in 1998. In the past few years the ENSDF data sets were updated considerably. However most of its update seems to steam from a large amount of experimental results related to high-spin nuclear physics. A quite common feature of this improvement is the lack of connections of the deformed bands to the ground state, which makes these updates less important for the purpose of low energy discrete library to be used in nuclear reaction calculations. Setup of the library generating codes and files for an easy and regular upgrade of the discrete level library was undertaken on the nds121 computer of the Nuclear Data Section. The NDS setup was used to produce the first update to the RIPL-2 discrete level scheme library using the 2004 October update of ENSDF and the NDS computer.

Introduction

The history of the Reference Input Parameter Library (RIPL) can be traced back to the start of RIPL-1 Coordinated Research Project (CRP) initiated by the Division of the Physical and Chemical Sciences of the International Atomic Energy Agency [1]. The aim of the library was to facilitate nuclear reaction model calculations for practical applications, especially in those cases where no measurements can be made. Naturally, where measured data exist can be used as benchmarks of the reaction models. In a subsequent CRP entitled as Reference Input Parameter Library Phase II (RIPL-2) started in 1998 aimed to test RIPL-1, but in the course some parts had to be improved substantially. One of them was the Discrete Level Scheme Library (DLSL). By the end of the CRP a completely new and enhanced DLSL was created from the ENSDF-II data set used in the update of Table of Isotopes [2]. The advantage of this data set over the original Evaluated Nuclear Structure Data File (ENSDF) was that it contained direct connections between the gamma transitions and their initial and final states. Because the update of Table of Isotopes seems to be slowed down we had to go back to the original ENSDF data set that is regularly updated at the Nuclear Data Center in Brookhaven National Laboratory.

The aim of this work is to produce an easy to use set of programs which can use the original ENSDF and creates the DLSL in the format that was defined in RIPL-2 [3].

Changes in the original programs

In the 3rd chapter of the RIPL-2 handbook a detailed description of the structure of the DLSL has been given. The DLSL structure was not changed during the update of the various FORTRAN programs. The procedure of the preparation of the DLSL was presented in ANNEX 3.F, which was slightly modified in the course of reprogramming. Instead of using the program *discretels.f90* twice, two versions were written and called *discretels1.f90* and *discretels2.f90*. This way batch running of the programs became easier. Screen drawing ability of levglobal.f90 was disabled, primarily because it was platform dependent. In the batch running the visual checking of the result is not possible, thus the program *cumcomp.f90* is left out from the package.

The largest change was done in the program *ensdf2read.f90*. As we have already mentioned the ENSDF-2 contains direct information on the initial and final state for each gamma transition. In the original ENSDF file this information is missing, thus a program part has had to be developed to re-build all of the decay schemes uniquely. These results were then put in the my.enx file in ENSDF-2 format. A lot of trouble was caused by the limitless variety of the notation of decoupled high spin bands (“X+0”, “X+”, “+X”, “0+X”, “X”). Many times they are placed after the last level with known energy value, but in a number of cases they are placed in the middle of the level scheme with known energies. Due to these extensive problems we have decided to remove all of these uncertain data from

the production of the updated DLSL files. The only case when the uncertain level was not removed happened when it was the first state of the data set. In this case the first level was considered to be the ground state. This assumption can be bad if this first level is followed by a second level with uncertain energy, which turn out to be an isomeric state and only the order of these two states are not known. To find out those nuclei, the file named as *stat_001_293.txt* can be studied. For the current update we present those cases for which the first levels are uncertain in Table 1:

A	Z	LevNo	GamNo	NoXdropped	S#Xfirst	Chi	A	Z	LevNo	GamNo	NoXdropped	S#Xfirst	Chi
55	30	1	0	0	1	0	184	83	1	0	1	1	0
60	23	1	0	3	1	0	186	81	1	0	8	1	0
68	25	1	0	0	1	0	188	81	1	0	8	1	0
76	29	1	0	1	1	0	188	83	1	0	1	1	0
86	41	1	0	79	1	0	190	81	1	0	24	1	0
90	43	48	87	2	1	0.532	190	83	1	0	2	1	0
94	45	1	0	2	1	0	193	84	1	0	4	1	0
97	48	1	0	0	1	0	194	85	1	0	1	1	0
98	49	1	0	1	1	0	196	86	1	0	0	1	0
102	37	1	0	0	1	0	206	89	1	0	2	1	0
102	39	1	0	10	1	0	219	91	1	0	0	1	0
102	41	1	0	14	1	0	220	91	1	0	0	1	0
110	45	1	0	7	1	0	235	95	1	0	0	1	0
112	45	1	0	5	1	0	239	97	1	0	1	1	0
119	47	1	0	4	1	0	246	97	1	0	0	1	0
120	57	1	0	0	1	0	246	99	3	0	0	1	0
124	57	1	0	42	1	0	246	101	1	0	0	1	0
126	57	1	0	37	1	0	253	103	1	0	2	1	0
130	59	1	0	152	1	0	253	104	1	0	1	1	0
134	59	1	0	87	1	0	254	101	5	0	1	1	0
135	61	2	0	31	1	0	262	107	1	0	1	1	0
136	61	1	0	104	1	0	265	104	1	0	0	1	0
136	63	1	0	1	1	0	267	108	1	0	1	1	0
138	51	1	0	0	1	0	267	110	1	0	0	1	0
138	65	1	0	0	1	0	268	109	1	0	0	1	0
144	53	1	0	0	1	0	269	108	1	0	2	1	0
148	69	1	0	0	1	0	269	110	1	0	0	1	0
151	71	1	0	0	1	0	271	110	1	0	1	1	0
156	61	1	0	0	1	0	272	111	1	0	0	1	0
172	75	1	0	10	1	0	273	110	1	0	1	1	0
173	77	1	0	47	1	0	277	108	1	0	0	1	0
177	69	1	0	0	1	0	277	112	1	0	0	1	0
178	73	1	0	20	1	0	281	110	1	0	0	1	0
181	81	1	0	1	1	0	285	112	1	0	0	1	0
181	82	1	0	0	1	0	289	114	1	0	0	1	0
184	71	1	0	1	1	0							
184	81	1	0	2	1	0							

TABLE 1 List of nuclei for which the first excited state is uncertain

Diagnostic files have been added to the ensdf2read.f90 program to record the problematic cases. In the file Diagnose_001_293.txt, the processed file names are written together with gamma rays for which the placement results in large Chi value. An example is given for 42K.

The portion of ENSDF that gives large Chi value for initial level of 4878.6(3) keV is:

```
42K   L 4878.6    3  (1+:4+)
42K X L XREF=FG
42K  CL J$G to 3+; primary G from 1+,2+
42K   G 1509.92   4   55    9
42K F G FL=3367.34
42K   G 3185.09   9   53    3
42K F G FL=1692.00
42K   G 3468.99   9  100    5
42K F G FL=1407.922
```

It triggered the following messages in the file *Diagnose_001_293.txt*:

```
Large Chi for gamma placement:        4.2
 4878.600  3367.340  1509.920     0.300     0.080     0.040
 42K   L 4878.6    3  (1+:4+)
 42K |f      G 1509.92   4   55    9
Large Chi for gamma placement:        4.4
  4878.600  1692.000  3185.090     0.300     0.040     0.090
 42K   L 4878.6    3  (1+:4+)
 42K |f      G 3185.09   9   53    3
Large Chi for gamma placement:        4.9
  4878.600  1407.922  3468.990     0.300     0.019     0.090
 42K   L 4878.6    3  (1+:4+)
 42K |f      G 3468.99   9  100    5
```

There are much larger discrepancies noted in *Diagnose_001_293.txt*, which are not shown here.

The other diagnostic file is *stat_001_293.txt*, which has been mentioned earlier. In this the number of levels and gammas were noted for all nuclei in the data set after the uncertain levels had been removed. The last column denotes the total normalized Chi values for the decay scheme reconstructions. There were cases where these were much larger than the expected value of 1. In this file the total number of the dropped +X, +Y, +Z … levels and the serial number of the first occurrence of +X, +Y, +Z … levels were also recorded for each nuclei. At its end the total number of rows (1903028) read in and the total number of nuclei (2923) found in the data set were also included.

There are many other diagnostics files, which are not mentioned here. They were mentioned in Ref. [3] or are adequately described in the FORTRAN codes.

Implementation and batch processing

The difference between the DIGITAL FORTRAN90 and the Lahey FORTRAN95 is rather small. The end of file function is missing in the Lahey FORTRAN, thus it had to be written. The IMSL library that is part of the DIGITAL FORTRAN90 is not presented in Lahey FORTRAN, thus related functionalities were replaced, for example the matrix inversion. Some other minor differences in representation, for example the random number generation, were also fixed.

One of the requests was to run the program by non-specialists. Batch processing provides the best solution for this problem. To achieve this, three scripts were written to run the programs in the right order under LINUX, equipped with Lahey FORTRAN facilities. These scripts are making of advantage of a strictly defined file structure. Six directories were set up. Four of them contain all of the necessary files to produce the final files. The directory names are:

ENSDF_files
necessary_files
prog_files
script_files
work
Doc

The **ENSDF_files directory** must contain the newest ENSDF data files with file name forms of *ENSDF.XXX*, where *XXX* means the mass number of different isotopes. The form of the numbers are 001, 002, … ,010, 011, … , XXX.

The **necessary_files directory** contains three predefined files. These are the *icctbl.dat* and *iccndx.dat*. The first is a binary file containing internal conversion coefficient (icc) data and the second is an index file for that table. The third file *stable2005.csv* contains information on the position of the line of stability.

The **prog_files directory** contains five executable program files that are producing all of the calculations, the data retrievals, the reformatting and the testing procedures, and produce the output files that make up the DLSL. The DLSL file names have the form of *ZYYY.dat*, wehre *YYY* is the charge number and it has similar format like the mass numbers *XXX*. The nuclear decay schemes with same charge numbers are printed in them in readable format as described in Ref. [3].

The **script_files directory** has three script files. The file named as *clean.script* deletes all of the non-executable files in the **work directory**. The **work directory** is intended for being a place to perform all calculations. The second script is named as *rdls.script*. It first copies all the necessary files to the **work directory**, and then runs all of the five executable FORTRAN programs, which create the final result. The running orders of the executables are defined in this script. The resulting DLSL files are written also to this directory together with the diagnostic and information files. The third script copies all of the executables to the **prog_files directory** from the four directories (**ensdf2read2005lh, discretel2005lh, levglobal2005lh** and **dtest2005lh**), in which one can make modification of the FORTRAN codes. To reflect the changes in the codes this copying step is important.

The documentation (this report) and an MS EXCEL file were copied in the **Doc directory**. The file names are *RIPL-X discrete level library.doc* and *parall_comparison.xls*. The current absolute location of the above directories is nds121.iaea.org *home/belgya/ripl3*.

Finally we should note that possible future changes in ENSDF record formats can not be excluded. These changes may cause malfunction during the running process of the programs. In this case the diagnostics files can help to find out the first place of the format changes that causes the malfunction.

Comparisons

To check that the new DLSL is reliable, one can compare the file called *parall.dat* to the previous versions. This contains the most important information for each isotope that was evaluated. Big changes in the parameters indicate some major action made in the new evaluation of the ENSDFs. The format of the *parall.dat* files is extensively described in Ref. [3]. An example of the comparison is given in the EXCEL file called as *parall_comparison.xls*. In this file the old version of *parall.dat* is loaded in the worksheet *parall*, and then the new version is loaded in the worksheet *parall2005*. A column contains the notation old and new was added to the two data sets respectively. In the comparison sheet both of the contents of the two worksheets were copied in to one table. This table can be sorted by the mass and charge numbers and by the creation time (old, new). This way the results of the old and the new evaluations of the same nucleus appear next to each other. The macro named *changes* creates a comparison of the two data sets in the worksheet *changes*. A new sorting by time can help to make three distinct categories, the completely new data, the old, which is not presented in the new, and a comparison. In this later the differences in the number and the maximum number (up to which the scheme is considered to be complete) of levels between the new and the old data set were calculated. Out of this analysis it was found that 323 new data sets of nuclei have appeared in the new ENSDF (dated as Oct. 2004) evaluation. Most of them are just having a ground state and they are not important for the DLSL library. There was only a handful with more than 9 levels that appeared in or disappeared from the new evaluation. They are listed in Table 2.

Z	A	Symbol	dNlev	dNmax	Umax	Time	Comments
23	48	V	82	42		new	Were missed by mistake from the old version
24	48	Cr	39	9		new	Were missed by mistake from the old version
43	89	Tc	40	16		new	
45	92	Rh	20	10		new	
67	141	Ho	11	1		new	
66	143	Dy	80	9		new	
73	174	Ta	26	8		new	
7	16	N	66	30		old	There is no adopted levels in the new data set
59	156	Pr	10	1		old	Missing from the new ENSDF.156 file

TABLE 2 Data changed from the new ENSDF evaluation.

Changes in the number of levels common in both evaluations can be represented as a histogram plot (see Fig. 1 below). It is especially interesting the case when there is a decrease in a number of levels. Most of these decreases are due to the drop of the uncertain levels (+X,+Y), but in some cases the evaluators decided to include less levels e.g. for ^{87}Kr nucleus. It can also be seen that in the past six years more new levels were put in the decay schemes than the amount has been lost due to the uncertain levels and other reasons.

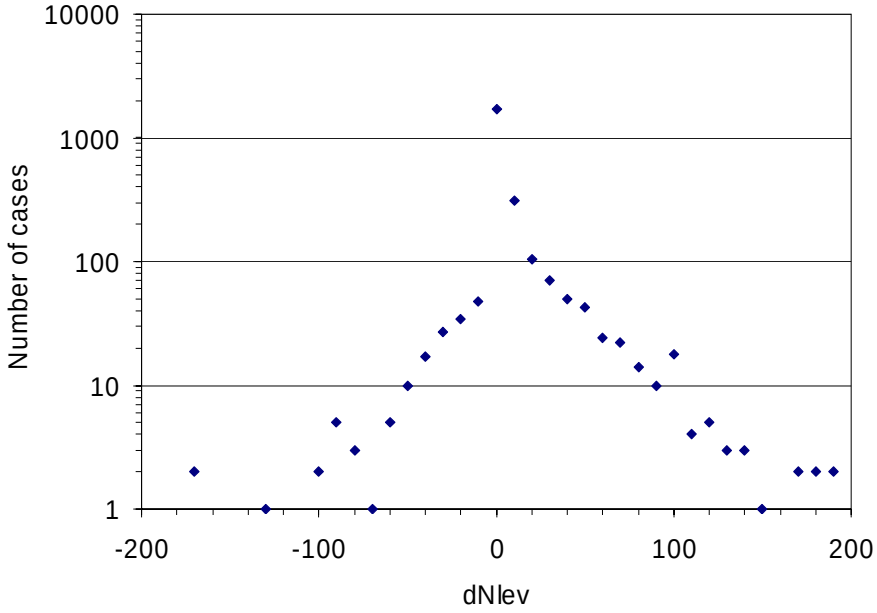

FIG. 1 Changes of number of levels in the new DLSL relative to the old DLSL.

It is also interesting to see that how the maximum level number or more meaningfully the maximum level energy was changed. This is shown in Figure 2.

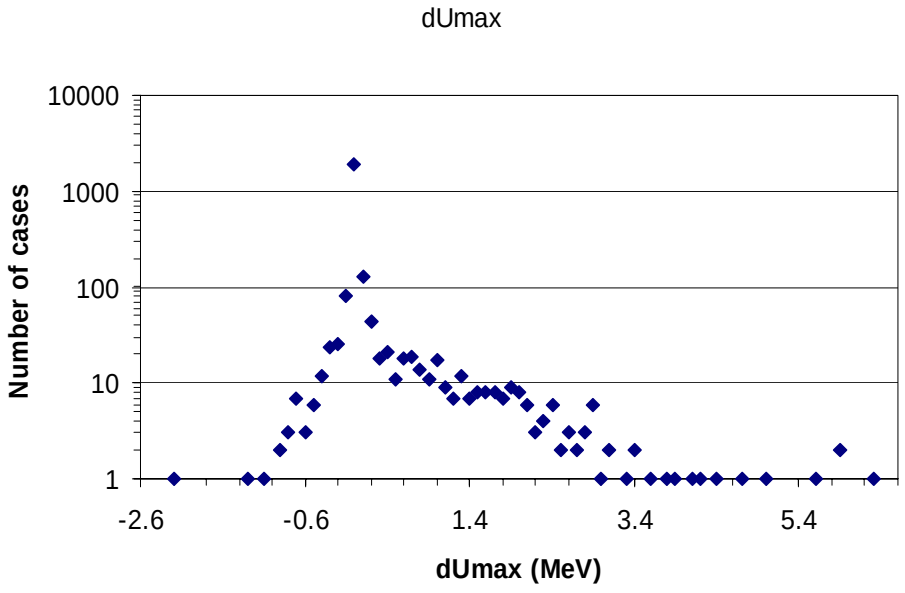

FIG 2 Changes of U_{max} of levels in the new DLSL relative to the old DLSL.

It can be seen that in the majority of cases (1942 out of 2547) no change has happened. On the other hand, due to higher number of new levels the U_{max} values increased for about 400 nuclei.

Finally, the comparison of the nuclear temperature functions T(A), obtained from fits to the

cumulative number of levels of a selected set of nuclei [3] for both the new and the old data sets are shown in Figure 3.

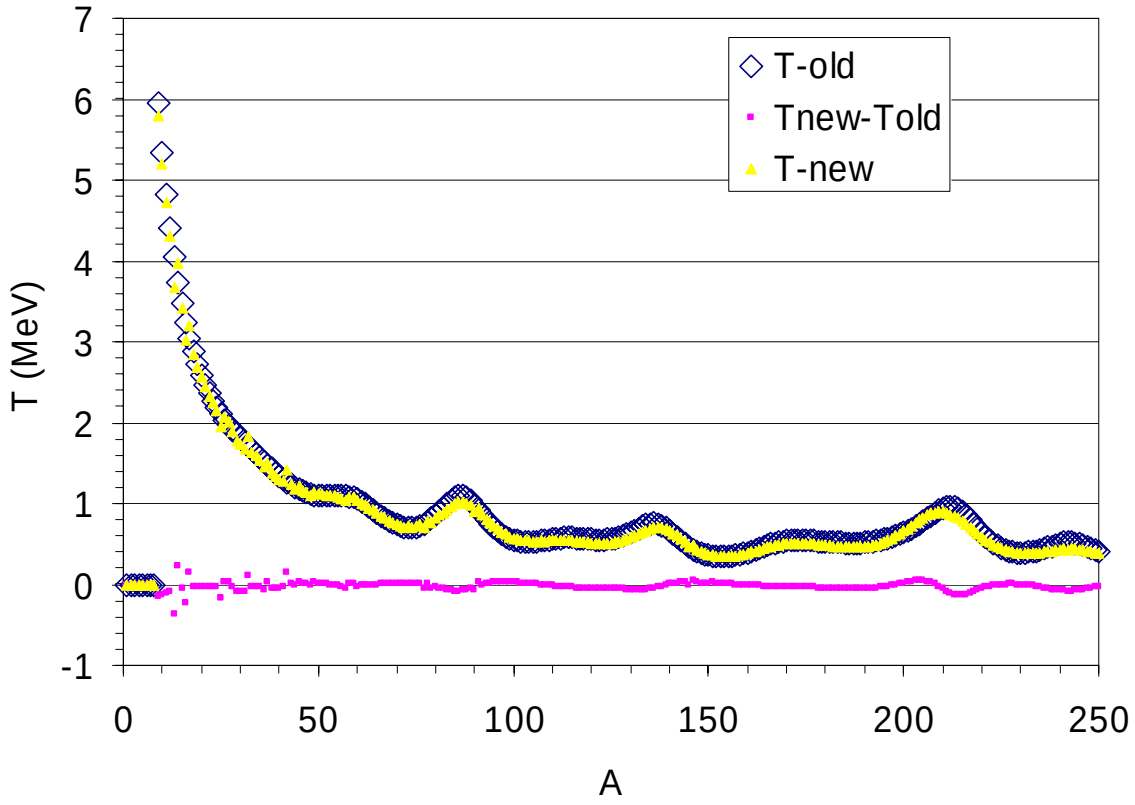

FIG 3 Comparison of the nuclear temperature fits to the old and new data.

We can say that the temperature fits were quite stable, did not change much for the new data set. Most of the changes occurred near to the closed shells. For the new fit the locations of the maxima seem to change closer to the magic numbers.

Recommendations to the ENSDF evaluators

The ENSDF data evaluators should find a better representation of the +X, +Y, +Z … level energy notations in ENDSF; especially when there is some hint that where the band head is located in the level scheme. This information should not be hidden in the comments, because it is impossible to handle by computer programs. It is better to have definite energies with large uncertainties for the band heads. The ones that are completely uncertain should be placed to the very end of the known energy levels, this way they can be easily separated. In case of close laying ground and first excited states for which isomer transition may exist should be handled separately from the high-energy, high-spin states. These low-laying isomer states can be important for cross section calculations.

There is a list of gamma rays and the corresponding initial and final levels in file *Diagnose_001_293.txt* for which the energy differences are larger than 4 sigma values. The evaluators at BNL should also study these problematic cases. Either the placement is wrong or the uncertainty estimation is in error.

An example for ^{41}K is given here (in the gamma line |f means that a flag was given for the final state; first line gives the interpreted energy for the initial and for the final levels, the gamma-ray energy, and their uncertainties):

```
/home/belgya/ripl3/ENSDF_files/ENSDF.041
Large Chi for gamma placement:     7297.3
  5496.610  4026.940  2968.610     0.070     0.070     0.180
 41K   L    5496.617  (7/2+)
 41K |f      G 2968.61   18 16     2
```

The corresponding original ENSDF portion is:

```
 41K   L 5496.61   7  (7/2+)
 41K X L XREF=JN
 41K  CL J$G's to 5/2+, 5/2- and 11/2+
 41K   G 887.13    5  5.3    16
 41K   G 1499.78   13 19     4
 41K   G 2784.08   17 20     2
 41K   G 2968.61   18 16     2
 41K F G FL=4026.94
```

In the listing in the file *stat_001_293.txt*, the last column gives the total Chi of the energy fitting of gamma rays in to the level scheme. If the Chi is large, there must be a corresponding problem in the file *Diagnose_001_293.txt.*

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References

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