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## Recommended Input Parameter Library (RIPL) for Fission Cross Section Calculation

Summary Report of the 1st Research Coordination Meeting (RCM)

IAEA Headquarters, Vienna, Austria
6-9 June 2017
Meeting Room VIC ME027

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IAEA, Vienna, Austria

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January 2018

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**Abstract**
A summary is given of the First Research Coordination Meeting on Recommended Input Parameter Library (RIPL) for Fission Cross Section Calculation. The new RIPL-4 library should serve as input for theoretical calculations of nuclear reaction data at incident energies up to 200 MeV, with a focus on reproducibility of nuclear model calculations as needed for energy and non-energy modern applications of nuclear data. Technical discussions and the resulting work plan of the Coordinated Research Programme are summarized, along with actions and deadlines.

January 2018

**CONTENTS**

## 1. Introduction

While experimental data provide extremely important constraints for evaluated data, it is well established that nuclear modelling is required to fill the gaps in measured data and make evaluated data files both complete and physically consistent. It has long been recognized that nuclear reaction theory as implemented in modern reaction codes (e.g., EMPIRE and TALYS) is believed to be in a position to meet most of the requirements for practical applications.

However, the major sources of uncertainty are the input parameters needed to perform theoretical calculations and reaction modelling. The International Atomic Energy Agency (IAEA) has worked extensively since 1993 on a library of recommended and validated nuclear-model input parameters, referred to as the Reference Input Parameter Library (RIPL). RIPL undertakes 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 completed in 2002 (**IAEA-TECDOC-1506**)[2]. Substantial improvements and extensions to the Starter File have been made; all files selected for RIPL-2 have been prepared in the unified format, which facilitates their use in the reaction codes. The last phase of the project, so far, was completed in 2008 with the production of the RIPL-3 database (https://www-nds.iaea.org/RIPL-3/). A comprehensive scientific report was published in the Nuclear Data Sheets in 2009 [3].

Some problems have been identified since the release of the RIPL-3 database, in particular, the lack of a comprehensive validation of RIPL input parameters for fission against available experimental data, therefore there is no guarantee of a reproducible and/or accurate calculation of fission cross sections. A large variability in calculated fission cross sections is observed due to the use of different fission formalisms, implementation in the codes, and/or combination of parameters. Fission cross sections are a key quantity for nuclear power applications, therefore, a Co-ordinated Research Project (CRP) on “Recommended Input Parameters for Fission Cross-Section Calculations” was recommended at the CM held at the IAEA headquarters in December 2015 (see report INDC(NDS)-0654, available at: https://www-nds.iaea.org/publications/indc/indc-nds-0654.pdf).

The First Research Coordination Meeting (RCM) of the RIPL-4 CRP was held at IAEA Headquarters, Vienna (Austria) from 6 - 9 June 2017 and attended by twelve CRP participants. The IAEA was represented by A. Koning (Head, Nuclear Data Section), P. Dimitriou,

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[1] Handbook for calculations of nuclear reaction data: Reference Input Parameter Library (IAEA, Vienna, Austria, 1998), IAEA-TECDOC-1034.
Available at: https://www-nds.iaea.org/publications/tecdocs/iaea-tecdoc-1034.pdf

[2] Handbook for calculations of nuclear reaction data: Reference Input Parameter Library RIPL-2 (IAEA, Vienna, Austria, 2006), IAEA-TECDOC-1506.
Available at: https://www-nds.iaea.org/publications/tecdocs/iaea-tecdoc-1506.pdf

[3] R. Capote, M. Herman, et al, “RIPL: Reference Input Parameter Library for Calculations of Nuclear Reactions and Nuclear Data Evaluations,” *Nuclear Data Sheets* **110** (2009) 3107-3214.

M. Verpelli and R. Capote, who served as Scientific Secretary. The approved Agenda is attached (Appendix I), as well as a list of participants and their affiliations with a group picture (Appendix II). S. Goriely was elected Rapporteur.

Prior to the meeting, the assignment of tasks related to each of the RIPL segments had been discussed by e-mail between the participants and Scientific Secretary. 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-3 database. Some changes are expected in order to accommodate additional inputs needed for fission cross-section calculations that have not been provided before.

### 1.1. Scope of the CRP

Recommend a comprehensive set of input parameters with estimates of uncertainties needed for modelling of fission cross sections based on microscopic and phenomenological approaches. Priority will be given to the modelling of photon and nucleon induced reactions on actinides and a description of relevant reaction channels with emphasis on incident energies below 30 MeV.

### 1.2. Model input parameters to be considered

*Fission parameters:*

Input parameters will be provided according to the following three descriptions of the fission path: fission barriers (parabolic), barrier and wells (parabolic), full 1D fission path (as in RIPL-3)

- Compilation of available sets of empirical fission barriers (heights and widths) used in reaction calculations.
- Compilation of available sets of class II/III states in the well(s) for accurate prediction of near threshold resonances.
- Compilation of available sets of transition states and tabulated level densities at the saddle points, and corresponding tabulated ground state level densities.
- Compilation of available sets of theoretical barriers (including symmetries) and comparison with recommended empirical set to assess the predictive power.

*Other input parameters:*

- Compilation of available sets of optical model potentials for actinides.
- Compilation of available sets of gamma-ray strength functions for actinides.
- Compilation of available sets of theoretical masses and ground state deformations.
- Update of sets of discrete levels and decay properties from ENSDF, NUBASE-2012.
- Update of average resonance properties for actinides (e.g. average spacing, strength function, $\Gamma\gamma$) if new evaluations are available.

### 1.3. Planned CRP outputs

- A technical document describing both the nuclear reaction formalism and model parameters included in the database.
- A database will be made available for online distribution. All recommended parameters have to be tested using model calculations and compared with available reaction data, their inclusion into the database should be justified.

### 1.4. Planned CRP Goals

1) The following input parameters will be included into the database:

*Fission parameters*

- Recommended set of empirical fission barriers (heights and widths) with estimated uncertainties.
- Recommended set(s) of theoretical barriers (including symmetries) and comparison with recommended empirical set to assess the predictive power.
- Recommended set(s) of class II/III states in the well(s) for accurate prediction of near threshold resonances for selected actinides (e.g. U-238, Th-232, Pa-231, etc.)
- Recommended set(s) of transition states and tabulated level densities at the saddle points, and corresponding tabulated ground state level densities.

*Other input parameters*

- Recommended set(s) of optical model potentials for actinides.
- Optimized sets of gamma-ray strength functions for actinides including renormalization coefficients to describe available experimental data.
- Recommended set(s) of theoretical masses and ground state deformations.
- Updated set of discrete levels and decay properties from ENSDF, NUBASE-2012.
- Updated set of average resonance properties for actinides (e.g. average spacing, strength function, etc.) if new evaluations are available.

2) Recommend sets of complete input parameter files for major codes optimized for the description (as coherent as possible) of available experimental cross sections for selected actinides (coherence means to try to obtain a unique set of fission input parameters for each fissioning nucleus independent of the fission chance and projectile). A typical input file may include fission barriers (including symmetries), class II/III states (and level densities) in the well(s) for accurate prediction of near threshold resonances, transition states and tabulated level densities at the saddle point, and corresponding ground state level densities.

## 2. Summary of Participants' Presentations

Participants' presentations are available at the IAEA website:
https://www-nds.iaea.org/index-meeting-crp/RIPL-4/RCM1/

### 2.1. Microscopic determination of fission observables

S. Goriely, J.-F Lemaître, S. Hilaire, N. Dubray, N. Martin

From the theoretical point of view, despite more than 70 years of research, fission is one of the least well understood processes in low-energy nuclear physics. In practical applications, it remains of major importance to be able to estimate accurately the probability in which fission occurs as well as the number of neutrons released during the fission process. Almost all existing evaluations of the fission observables rely on the multiple-humped fission penetration model where barriers are described by inverted decoupled parabolas. Such approaches consider all ingredients as free parameters in order to be able to achieve more or less accurate fits to experimental cross sections. Although such adjustments respond to the needs of crucial nuclear applications (in particular, nuclear energy production and nuclear waste transmutation), their predictive power remains poor due to the large number of free parameters and, therefore, these methods cannot be used in applications requiring a purely theoretical description of fission for experimentally unknown nuclei, such as nuclear astrophysics.

Recent studies aim at providing sound descriptions of some of the basic nuclear ingredients required to describe fission cross sections [1-6], and in doing so to avoid the phenomenological aspect of most of the fission studies up to date. It is now possible to use the microscopic quantum mechanical approach starting from the sole Gogny or Skyrme effective nucleon-nucleon interaction as input to model the fission process. Within a semi-microscopic framework based on the Skyrme effective interaction with phenomenological collective corrections, potential energy surfaces and static fission paths have been computed systematically [3,6] and included in the RIPL-3 database. Nuclear level densities have also been calculated both in the ground-state, fission saddle points and super-deformed minima within the HFB plus combinatorial model on the basis of the same Skyrme interaction.
Similar calculations will be performed on the basis of the finite-range Gogny interaction [7-9] and the corresponding potential energy surfaces used for cross section calculation [7, 9-11]. Such a state-of-the-art approach has shown its ability to reproduce several important features of fission [10-11]. This latter approach will be used in large-scale calculations to improve the reliability of the predictions for all the neutron-rich nuclei of interest in practical nuclear applications.
More precisely, such a new determination of the potential energy surfaces and corresponding fission paths will be used to estimate, on the basis of microscopic fission ingredients, the fission transmission coefficient, a quantity of first importance in the determination of the neutron-induced, beta-delayed and spontaneous fission rates.

The starting point of the present research project is the calculation of the energy surfaces on the basis of the D1M Gogny interaction [8] that will be performed in collaboration with the Bruyères-le-Chatel research team. It includes the following steps:

- The fission barriers height will first be calculated and compared with so-called experimental fission barriers to validate the accuracy of the model. The dynamical propagation of the compound system wave function in the potential energy surface will allow us to estimate the impact of the discontinuities on fission observables.
- The nuclear level densities at the corresponding saddle points and shape isomers will be estimated on the basis of the combinatorial approach, in the very same way as for the ground-state.
- The fission paths for all the $Z \geq 90$ nuclei will be included in the nuclear reaction codes TALYS to estimate the fission transmission coefficients on the basis of an improved description of the barrier penetration and newly determined nuclear level densities at the corresponding saddle points and shape isomers. This new miscroscopic input will be used to compute neutron-induced fission cross sections, as well as spontaneous and β-delayed fission rates in a coherent framework using the same D1M interaction. Our predictions will be compared with experimental data and those obtained with the Skyrme effective interaction [1-3] to test the predictive power of both approaches and their differences in the extrapolation far away from stability.

[1] S. Goriely, European Physical Journal A **51** (2014) 22 :1-21.
[2] S. Goriely, G. Martinez Pinedo, Nuclear Physics A **944** (2015) 158.
[3] S. Goriely, M. Samyn, J.M. Pearson, Physical Review C **75** (2007) 064312.
[4] S. Goriely, et al., Physical Review C **79** (2009) 024613.
[5] S. Goriely, et al., Physical Review C **83** (2011) 034601.
[6] R. Capote, et al., Nuclear Data Sheets **110** (2009) 3107.
[6] J.-F. Berger, M. Girod, and D. Gogny, Nuclear Physics A **428** (1984) 23c.
[7] J.-F. Berger, M. Girod, and D. Gogny, Computer Physics Communication **63** (1991) 365.
[8] S. Goriely, S. Hilaire, M. Girod, S. Péru, Physical Review Letters **102** (2009) 242501.

[9] H. Goutte, et al., Physical Review C **71** (2005) 024316.
[10] N. Dubray, H. Goutte and J.P. Delaroche, Physical Review C **77** (2008) 014310.
[11] N. Dubray and D. Regnier, Computer Physics Communications **183** (2012) 2035.

### 2.2. Nuclear Fission Barriers from MultiDimensionally-Constrained Covariant Density functional Theory

Shan-Gui Zhou

Many different shape degrees of freedom play crucial roles in determining the nuclear ground state and fission properties. To study nuclear potential energy surfaces, it is desirable to have microscopic and self-consistent models in which all known important shape degrees of freedom are included. By breaking both the axial and the spatial reflection symmetries simultaneously, we developed multi-dimensionally constrained covariant density functional theories (MDC-CDFTs) [1-4]. The nuclear shape is assumed to be invariant under the reversion of $x$ and $y$ axes, i.e., the intrinsic symmetry group is $V_4$ and all shape degrees of freedom $\beta_{\lambda\mu}$ with even $\mu$, such as $\beta_{20}$, $\beta_{22}$, $\beta_{30}$, $\beta_{32}$, $\beta_{40}$, etc., are included self-consistently.

The MDC-CDFT consists of two types of models: the multidimensionally constrained relativistic mean field (MDC-RMF) model [12] and the multidimensionally constrained relativistic Hartree-Bogoliubov (MDC-RHB) model [3]. In the MDC-RMF model, the BCS approach has been implemented for the particle-particle (pp) channel. In the MDC-RHB model, pairing correlations are treated by making the Bogoliubov transformation.

The MDC-CDFT’s have been applied to the study of fission barriers and potential energy surfaces of actinide nuclei [1,2,5,6], third minima in potential energy surfaces of light actinides [7], shapes and potential energy surfaces of superheavy nuclei [8], the $Y_{32}$ correlations in $N$ = 150 isotones [9] and Zr isotopes [3], and the shape of hypernuclei [10,11]. In this talk I will introduce MDC-CDFT's and applications on fission barriers.

We have obtained the PES’s of actinide nuclei in three-dimensional deformation space, i.e., $E = E(\beta_{20}, \beta_{22}, \beta_{30})$, with the MDC-RMF model. It was found that for the second fission barriers (the outer one in many cases) in these actinides, the triaxial shape is very crucial. Both the second barrier and the first one are lowered considerably due to the triaxial distortion as compared with results from axially symmetric calculations. This lowering effect for the reflection-asymmetric outer barrier is 0.5~1 MeV, accounting for 10%~20% of the barrier height. With the triaxial deformation considered, a better agreement with empirical values of the outer barrier heights in actinide nuclei was found. By examining these PES’s, one can learn a lot of interesting and useful information concerning the shape and stiffness of the ground and isomeric states, the fission barrier heights and the lowering effect of triaxial and octupole deformations on fission barriers.

Furthermore, two-dimensional PES’s of $^{226,228,230,232}$Th and $^{232,234,236,238}$U are mapped and the third minima on these surfaces are located. Then one-dimensional potential energy curves along the fission path are analysed in detail and the energies of the second barrier, the third minimum, and the third barrier are determined. The functional DD-ME2 predicts the occurrence of a third barrier in all Th nuclei and $^{238}$U. The third minima in $^{230,232}$Th are very shallow, whereas those in $^{226,228}$Th and $^{238}$U are quite prominent. With the functional PC-PK1 a third barrier is found only in $^{226,228,230}$Th. Single-nucleon levels around the Fermi surface are analysed in $^{226}$Th, and it is found that the formation of the third minimum is mainly due to the

$Z$ = 90 proton energy gap around $\beta_{20}$ = 1.5 and $\beta_{30}$ = 0.7. It was concluded that the possible occurrence of a third barrier on the PES's of actinide nuclei depends on the effective interaction used in multidimensional CDFT calculations. More pronounced minima are predicted by the DD-ME2 functional, as compared to the functional PC-PK1. The depth of the third well in Th isotopes decreases with increasing neutron number. The origin of the third minimum is due to the proton $Z$ = 90 shell gap at relevant deformations.

In Recommended Input Parameter Library for Fission Cross Section Calculations (RIPL-4), a systematic study of potential energy surface of all actinide nuclei, including even-even, odd-$A$, and odd-odd ones, will be studied in detail with the MDC-RMF model. Comparison will be made with available empirical heights of fission barriers and predictions will be given for those nuclei which have not been studied experimentally. The importance of various shape degrees of freedom on fission barriers will be investigated. Associated quantities, e.g., transition levels, shell and pairing corrections at saddles, will be also studied.

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References:

[1] B. N. Lu, E. G. Zhao, and S. G. Zhou, Phys. Rev. C **85** (2012) 011301(R).
[2] B. N. Lu, J. Zhao, E. G. Zhao, and S. G. Zhou, Phys. Rev. C **89** (2014) 014323.
[3] J. Zhao, B. N. Lu, E. G. Zhao, and S. G. Zhou, Phys. Rev. C **95** (2017) 014320.
[4] S. G. Zhou, Phys. Scr. **91** (2016) 063008.
[5] J. Zhao, B. N. Lu, T. Nikšić, and D. Vretenar, Phys. Rev. C **92** (2015) 064315.
[6] J. Zhao J, B. N. Lu, T. Nikšić, D. Vretenar, and S. G. Zhou, Phys. Rev. C **93** (2016) 044315.
[7] J. Zhao, B. N. Lu, D. Vretenar, E. G. Zhao, and S. G. Zhou, Phys. Rev. C **91** (2015) 014321.
[8] X. Meng, et al., in preparation.
[9] J. Zhao, B. N. Lu, E. G. Zhao, and S. G. Zhou, Phys. Rev. C **86** (2012) 057304.
[10] B. N. Lu, E. G. Zhao, and S. G. Zhou, Phys. Rev. C **84** (2011) 014328.
[11] B. N. Lu, E. Hiyama, H. Sagawa, and S. G. Zhou, Phys. Rev. C **89** (2014) 044307.

## 2.3. Properties of actinides nuclei within macroscopic-microscopic Warsaw model

M. Kowal

Selected properties of even-even actinides nuclei obtained within the microscopic-macroscopic method developed by our Warsaw group were presented during the CRP meeting. Our model is based on the deformed Woods-Saxon single-particle potential in the microscopic part where the Strutinski shell correction method is applied and on the Yukawa-plus-exponential method in the macroscopic part. The residual pairing interaction is treated fully microscopically by solving BCS equations. To find saddles on multidimensional grids we are using a conceptually simple and at the same time very efficient - from a numerical point of view - technique, namely the Imaginary Water Flow (IWF) method.

1. It was shown that without any special adjustable parameters our calculated first and second fission barrier heights are in quite good agreement with existing experimental/empirical data. The largest discrepancy between our calculated fission

barriers and the data is less than 1.4 MeV for second ones and less than 1.0 MeV in the case of the first ones. The average discrepancy is respectively about 0.6 MeV and 0.4 MeV. The root mean square deviation has the value about 0.7 MeV for second and 0.5 MeV for first fission barriers. Thus, the agreement with the experiment is better than for the other theoretical calculations.

2. It has been demonstrated that the inclusion of triaxial shapes significantly reduces the fission barriers by up to 2.5 MeV.
3. The well-known effect of the mass asymmetry on the second barrier in actinides has been fully confirmed.
4. Our attempt to study a possible coexistence of the nonaxiality with mass-asymmetry in the second saddle suggests that its influence on the barrier is negligible.
5. The excitation of the second minima in actinides is systematically slightly underestimated (by 200-850 keV) in our model. Still, this is in much better agreement with data than those achieved by various Skyrme density functionals for which, depending on the choice of the interaction, differences between theoretical and excitation energy of the second minimum can be as high as 4 MeV.
6. It has been demonstrated that the inclusion of higher multipolarities can lead to a significant change of the fission path in the multidimensional deformation space and can consequently cause a considerable change of the fission half-lives.
7. The existing theoretical evaluations of fission barriers differ significantly. Even the results of the two models based on the microscopic-macroscopic approach differ dramatically for some nuclei.
8. We have also studied the existence of third, hyperdeformed minima in a number of even-even Th, U and Pu nuclei. Deep (3÷4 MeV) minima found previously by Ćwiok et al. are found spurious after sufficiently general shapes are included. A modification of the energy landscape by including $\beta_{10}$ is decisive. Since dipole is the first spherical harmonic in the radius expansion, one can suspect its pronounced effect. Indeed, that effect is significant. Not only the height of the third saddle is clearly reduced, but the whole landscape changed. The result indicates a large effect of new shapes, unattainable previously. Shallow third wells may exist in $^{230;232}$Th, with IIIrd barriers $\leq$ 200 and 330 keV (respectively). Now, an understanding of experimental results on the apparent third minima in uranium becomes an issue.

We are going to extend this approach on odd and odd-odd actinide nuclei. Adiabatic potential energy surfaces will be calculated by a minimization over configurations with one blocked neutron or/and proton on a level from the 10-th below to the 10-th above the Fermi level. In such a way, we will have the masses, pairing energies, shell corrections and deformations at all global and local minima as well as at all competing saddle points for actinides including odd systems. This coherent and comprehensive set of data can be used as the input fission parameters needed for modeling of fission cross sections.

## 2.4. Fission Barriers from 5-Dimensional Potential Energy Surfaces

Nicolae Carjan, Roberto Capote

The method of calculating potential energy surfaces of deformation is presented. The microscopic – macroscopic approach [1] is used:

$$E_{def}(\text{shape}) = E_{def}^{LD}(\text{shape}) + \delta E(\text{shape}), \tag{1}$$

with

$$\delta E = \sum_{n,p} \left[ \delta E_{shell}^{(n,p)} + \delta E_{pair}^{(n,p)} \right]. \tag{2}$$

The summation in (2) is carried out over the protons ($p$) and neutrons ($n$). The $E_{def}^{LD}$ (1) is the macroscopic liquid-drop deformation energy.

In this work, the nuclear shapes are defined in terms of modified Cassinian ovals [2].

$$R(x) = R_0[1 + \sum_n \alpha_n P_n(x)] \tag{3}$$

Besides the elongation parameter α two other most relevant shape parameters are included: $\alpha_1$ (the mass asymmetry) and $\alpha_4$ (the neck radius). In addition, the minimization of the deformation energy with respect to $\alpha_3$ and $\alpha_6$ is performed.

The saddle points and the minima of these 5 dimensional potential energy surfaces will be found by the immersion method. The corresponding total energies, shell and pairing corrections will be tabulated.

References

[1] M. Brack, J. Damgaard, A.S. Jensen, H.C. Pauli, V.M. Strutinsky, C.Y. Wong, Rev. Mod. Phys. **44** (1972) 320.

[2] V. Pashkevich, Nucl. Phys. A **169** (1971) 275.

## 2.5. Coupled-Channel Optical Model Potential for Even-Even Minor Actinides Using Extended Couplings

E.Sh. Soukhovitski, R. Capote, D. Martyanov, J.M. Quesada, S. Chiba

The goal is the development of optical model potential for even-even and odd minor actinides using extended couplings. Some time ago we suggested extension of coupled-channels (CC) optical model allowing coupling of levels from other than ground state band levels for both even-even and odd actinides [1]. On this basis, we developed an optical model potential describing simultaneously experimental optical data for $^{232}$Th, $^{233}$U, $^{235}$U, $^{238}$U, $^{239}$Pu. The weak point of such an approach is the necessity to adjust "effective deformations" for interband coupling, which is only possible for experimentally well investigated actinides. Our approach proved that the saturated coupling can be achieved only if levels of other than GS band levels are accounted for in even-even actinides. For odd actinides, the coupling saturation can be achieved by coupling only GS band levels.

Later we included additional coupling due to nuclear volume conservation during shape oscillations of soft non-axial even-even actinides [2]. Such a theory extension along with the used dispersive Lane-consistent optical potential parameters allow the best fit of all the optical experimental data for $^{238}$U and $^{232}$Th (total, angular distributions of scattered nucleons and angular distributions of neutrons with excitation of IAS and very accurate $^{238}$U to $^{232}$Th total

cross section ratio) up to 200 MeV nucleon incident energies. “Effective” deformations determining coupling strength were determined from soft-rotator model, with nuclear Hamiltonial parameters adjusted to describe low-lying collective levels from ground state, $\beta$-, $\gamma$-, negative parity, and $K$~2 bands. It is worth to mention, that building coupling strength we considered shape oscillations around $\beta_{20}$ $\beta_{30}$ equilibrium deformations while shapes determined by $\beta_4$ $\beta_6$ had been considered rigid.
During the first year of activity within this Project we applied a developed approach to $^{240}$Pu and $^{242}$Pu, the only actinides except $^{238}$U to $^{232}$Th with available experimental optical data above resonance energy region, and showed that it works for them. Moreover, we showed for all these actinides isotopes, that using theoretically predicted $\beta_4$ and $\beta_6$ predicted by FRDM12 [3] or WS4 [4] and adjusting $\beta_{20}$ to describe experimentally measured strength function $S_0$ allows to describe optical data from 1 keV. Without $\beta_{20}$ adjustment (using above mentioned theoretical estimates) we describe optical data from 100keV. Using WS4 [4] deformations in both cases describes experimental angular distributions much better, also these deformations are closer to the ones adjusted to describe experimental data.
A similar approach has been applied to all minor actinides experimental level schemes which allows determination of their soft-rotator nuclear Hamiltonian parameters, and we recommend predictions of optical data for them using our optical potential suggested at ND2016 [2] with deformations predicted by WS4 [4]. In case such actinides have experimentally measured strength function $S_0$ we adjust $\beta_{20}$to reproduce the latterwhich improves optical prediction as described in Ref. [5].
At the moment, we are on the way of applying the same approach to odd actinides. As has been shown before, in case of odd actinides coupling built on GS levels is enough for saturation, so any model describing other band levels is not needed. To account for the volume conservation we consider odd actinide nuclear volume to be the volume of its even-even core plus unpaired nucleon.

All described approaches are incorporated in the latest version of the OPTMAN code, which will be available from the RIPL data base with the produced inputs.

[1] E. Soukhovitskii, R. Capote, J.M. Quesada, S. Chiba, and D.S. Martyanov, Nucleon scattering on actinides using a dispersive optical model with extended couplings, Phys. Rev. C **94** (2016) 064605.
[2] D. Martyanov, E. Soukhovitskii, R. Capote, J.M. Quesada, and S. Chiba, Optical Model with Multiple Band Coupling Using a Soft Rotator Model, ND2016, *EPJ Web of Conference, (in print);*
[3] P Moeller, A. J. Sierk, T. Ichikawa, and H. Sagawa, Nuclear ground state masses and deformations: FRDM(2012), Atom. Data & Nucl. Data Tables 109-110 (2016) 1-204.
[4] N. Wang, M. Liu, Y.G. Deng, X.Z. Wu, and J. Meng, Surface diffuseness correction in global mass formula, Phys. Lett. B **734** (2014) 215-219 and N. Wang, M. Liu, X. Wu, Nuclear mass predictions with radial basis function approach, Phys. Rev. C **84** (2011) 014333.
[5] D. Martyanov, E. Soukhovitskii, R. Capote, J.M. Quesada, and S. Chiba, Predicting the optical observables for nucleon scattering on even-even actinides, , Chinese Phys C **41** (2017) 094105.

### 2.6. Introduction of CCONE code

Osamu Iwamoto, JAEA, Japan

An outline of the nuclear reaction modeling code CCONE was presented. The CCONE code was developed for evaluation of the JENDL project. It consists of optical model (spherical one, coupled-channel model and DWBA), pre-equilibrium exciton model, and Hauser-Feshbach statistical model. Formulations of fission modeling such as fission barrier penetrability and level density above saddle were shown. Some results of fission and capture cross sections for major actinides were presented.

Improvements of CCONE for calculation of reactions at higher induced energies were shown. They include multi-particle emission from the pre-equilibrium process and cluster emissions of the Iwamoto-Harada model. Calculated results of emission spectra of neutrons and alpha-particles are significantly improved.

A systematics formulation of prompt fission neutron spectrum (PFNS) was presented. It was developed based on the Los Alamos model by adjusting model parameters to PFNS experimental data for neutron induced and spontaneous fission of actinides. Results shows good agreements with experimental data.

## 3. Fission barrier & NLD calculations (Updated RIPL-3 Fission Segment)

### 3.1. Theoretical fission barriers & NLD

- RMF from Zhou (2$^{nd}$ RCM):
    - Static fission path along quadrupole deformation, including deformations, triaxial energy correction, inertial mass (total)
    - Fission barriers and deformation of saddle points and wells
    - Shell and pairing corrections at saddle points

      for Th to Cm along β-stability line (e-e, odd-A and odd-odd nuclei).

- Gogny HFB from Goriely & Hilaire (2$^{nd}$ RCM):
    - Static fission path along quadrupole deformation, including deformations, triaxial energy correction, inertial mass (total)
    - Fission barriers and deformation of saddle points and wells

      for Th to Ds from β-stability line to neutron-drip line (even & odd nuclei)
    - NLD at the GS and saddle points in a table format

- Mic-Mac models from Kowal:
    - Mass of the GS (June 2018)
    - shell and pairing corrections and deformations for GS and saddle points (June 2018)
    - energy excitations of superdeformed minima (2$^{nd}$ RCM)
    - spins and parities for odd nuclei GS (June 2018) and transition band-heads (2$^{nd}$ RCM)
    - Adiabatic fission barriers and widths (2$^{nd}$ RCM)

      for Th to Z=126 with N~136-192 (Cf) to N~160-192 (Z=126) by end of CRP (for 2$^{nd}$ RCM, major actinides only)

- Mic-Mac models from Carjan & Capote ($2^{nd}$ RCM):
    - Mass of the GS
    - Shell and pairing corrections and deformations for GS and saddle points
    - Adiabatic fission barriers and widths
      for Th to Cm along β-stability line

- Mic-mac model from Yavshits ($2^{nd}$ RCM)
    - Shell and pairing corrections and deformations for GS and saddle points
    - Adiabatic fission barriers and widths
      for W to Z=96 on a wide range around the β-stability line

- FRLDM fission barriers from Möller et al. (2008) to be provided by Kawano ($2^{nd}$ RCM)

- ETFSI fission barriers from Tondeur et al. (1998) to be provided by Goriely ($2^{nd}$ RCM)

- TF fission barriers from Myers & Swiatecki (1999) to be provided by Goriely ($2^{nd}$ RCM)

Special attention will be paid to some priority cases: major actinides ($^{236}$U, $^{239}$U, $^{240}$Pu), triple-humped cases ($^{233}$Th, $^{232}$Pa, $^{235}$U, $^{237}$U)

### 3.2. Nuclear level densities at saddle points

For each reaction code (EMPIRE-Sin, TALYS-Hilaire, COH3-Kawano, CCONE-Iwamoto, FUNF-Han), detailed information will be provided by Jan. 2018 for the GS and the saddle points about

- the default NLD prescription.
- the global default parametrization.
- a numerical NLD table for 3 reference cases ($^{240}$U, $^{247}$Pu, $^{244}$Np) in a defined U- and J-grid (plus parity if need be) for GS and saddles.
- the default discrete transition band-heads, if any.

By Jan. 2018 S. Hilaire will centralize the NLD prescriptions used in fission calculations and propose a common description for the $2^{nd}$ RCM to be assessed in fission cross section calculation after the $2^{nd}$ RCM.

The parameters to be used (including shell corrections, pairing, moment of inertia, …) will be discussed at the $2^{nd}$ RCM, also in view of consistency of the nuclear structure data provided in this CRP, both from mic-mac and mean-field models and ultimately tested in NLD and cross section calculations after agreeing on a common NLD prescription.

### 3.3. Empirical fission barriers & widths & NLD

Empirical fission barriers and widths to be provided by the $2^{nd}$ RCM

- RIPL-3 compilation (Capote)
- JENDL-4 fission barriers and widths (no uncertainties) (Iwamoto)
- Empire-specific fission barriers and widths for U (and Pu) isotopes (including uncertainties) (Sin)

For each set, detailed information will be provided by the 2nd RCM on

- the NLD prescription and parameters, together with a numerical NLD table for 3 reference cases ($^{238}$U, $^{239}$Pu, $^{238}$Np) in a defined U- and J-grid (plus parity if need be) for GS and saddles.
- The framework used for fission calculation (full damping, etc…)
- Discrete transition band-heads
- Optical potential

### 3.4. Discrete transition states

Empirical prescription for discrete transition states will be provided by the 2nd RCM

- For odd-A and odd-odd nuclei, the band-heads can be estimated from the single-particle levels at the saddle points and deduced from mic-mac (Kowal, Carjan) and mean-field (Hilaire).
- For even-even nuclei, exploratory deformed QRPA calculations constrained at the saddle point can be tested (Hilaire) as well as a 2-center shell model (Zhou). Feedback for the 2nd RCM

## 4. Cross Section Calculation

### 4.1. Test of nuclear input in cross section calculations

*First step for 2nd RCM by code authors* (EMPIRE-Sin, TALYS-Hilaire, COH3-Kawano, CCONE-Iwamoto, FUNF-Han)

- To perform a code intercomparison with "realistic" NLD input for $^{238}$U and $^{239}$Pu (cf ND2016 and IAEA 0654-INDC report). The NLD will be taken from HFB+Combinatorial method (RIPL3) where the $f_{sym}$ enhancement factor is embedded (Capote to prepare the file);
- The GS NLD to be recommended will be tested in radiative capture cross sections;
- Comparison of the OM cross section with Soukhovitski potential (RIPL-2408: ECIS-compatible dispersive rigid rotor with minimum 7 cc levels) that will be included in TALYS (Koning & Capote), CCONE (Iwamoto) and COH3 (Kawano) as well as in EMPIRE/OPTMAN (Capote) and tested; Details about the RIPL-2408 can be found in *Capote et al., Journal of Nuclear Science and Technology 45, 333 (2008)*; see ND2007 conference proceedings.
- The GS and saddle point NLD will be tested in first-chance fission cross sections and an intercomparison between the 5 codes will be done;
- The input from mean-field and mic-mac models will be included in the fission and NLD inputs for fission cross section calculations and a first test performed on $^{238}$U and $^{239}$Pu. These include fission barriers, widths (or fission path), deformations, shell corrections, pairing strengths, moment of inertia, transition bandhead spectra at saddle points (deadline: Nov. 2018).

*Second step after the 2nd RCM by code authors* (EMPIRE-Sin, TALYS-Hilaire, COH3-Kawano, CCONE-Iwamoto, FUNF-Han)

- Based on the commonly agreed NLD prescription and CRP barriers, some parameter tuning will be performed to provide "decent" fission cross section within typically ~20% (if possible) with respect to *evaluated* cross sections (based on experimental data).

- From the tested cases on $^{238}U$ and $^{239}Pu$, the input parameters will be tested for all fission cross sections experimentally available. If need be, additional tuning of the input prescriptions and parametrization will be performed.
- Systematics for fission inputs will be proposed and tested.
- Tables of fission paths and level densities from mean-field models will be renormalized after comparison with experimental data, if possible.

The 2nd CRP meeting will take place on Jan. 21-25, 2019 in Vienna

The file format will follow as much as possible the RIPL-3 format (.dat and .readme files) and be extended when needed.
A general review for a need to improve the RIPL format will be discussed at the 2nd RCM.
A request is already made to improve the format of OMP files by including the "E" for the power exponent.

## 5. Update of RIPL-3 Segments

### 5.1. Update of the Mass segment (Coord : S. Goriely)

It is proposed to include in RIPL-4:

- AME'16 experimental and recommended masses
- FRDM'12 instead of FRDM'95 (masses and deformations)
- HFB-27 masses and densities instead of HFB-14 (plus deformations)
- D1M masses, deformation and densities
- WS4 masses & deformations ($\beta_2$, $\beta_4$, $\beta_6$)

This proposal will be revisited at each RCM for new possible updates.

In addition, some local mass predictions in the heavy-superheavy regions are available from

- Warsaw model (M. Kowal) from Pb to Z=126 (1300 nuclei) (including deformations)
- Iterative GK model (S. Yavshits) from Z=1 up to Z=94
- Generalized GK model (S.-G. Zhou) from A=16 to A=250

These models will be assessed by their authors through mass model comparison and maybe at some point on fission cross section calculations.

### 5.2. Update of the Level segment (Coord: Capote)

Data sources: ENSDF, Calculated quantities, NUBASE

- Calculated quantities include spin and parity, gamma end-level energy, internal conversion factor, level after which the statistical density starts, some isomer energies
- "+X" level-energies (1100 "+X" bands involving some 16000 levels): using NUBASE and AME, the "+X" is assigned when a NUBASE-ENSDF isomer match is found on spin, parity, half-lives
  → 30% of the "+X" bands were fixed, the others were removed
- Level having same energy are split by 0.1k
- Levels after a gap larger than 8 MeV or 4.5x30/$A^{0.67}$ MeV are removed → the relevance of removing these levels from the Level file or leaving the code developer to make the appropriate cut still need to be assessed by the code developers for the next RCM (A. Koning, O. Iwamoto, T. Kawano, R. Capote).

- Bands are reported
- All decay models are presented
- Isomers ordering from NUBASE
- Sn and Sp from AME are included
- Holes in the ENDSF chart are filled with NUBASE nuclides

### 5.3. Update of the Resonance segment (Coord: Capote)

There will be a new compilation of resonance data from Mughabghab “soon”. R. Capote will compare these new resonance data with RIPL-3 and update RIPL-4 resonance file accordingly.

### 5.4. Update of the Optical Model segment (Coord. Capote)

New potentials will be included:

- Charged-particle spherical optical potential from Y. Han
- The updated Soukhovitski potential for actinides (as a code)
- Kunieda’s potential (by. R. Capote)
- High-energy potential by S. Yavshits

This update will be revisited at the next RCM.

### 5.5. Update of the Level Density segment (Coord: Hilaire)

No new fundamental NLD models have been proposed since RIPL-3. There are already far too many options in RIPL-3. For fission, we need to consider the same methods for both the GS and saddle points.
Since new Gogny-HFB plus combinatorial calculations of the NLD at the saddle points will be provided for RIPL-4, new tables for the GS will also be provided.

From the code developers and data evaluators, the NLD to be recommended can be tested during this CRP. One common NLD analytical prescriptions could be proposed for all code developers to be included in RIPL-4.

S. Hilaire will centralize the NLD prescriptions used in fission calculations (EMPIRE, TALYS, COH3, CCONE, FUNF) and propose a common description to be assessed after the next RCM.

The parameters to be used (including shell corrections, pairing, moment of inertia, …) will be discussed at the next RCM, also in view of consistency of the nuclear structure data provided in this CRP, both from mic-mac and mean-field models and ultimately tested in NLD and cross section calculations after agreeing on a common NLD prescription.

### 5.6. Update of the Gamma-ray strength function segment (Coord: Demetriou)

There is a full CRP on photon strength function (2016-2020) that will provide recommended strength functions, not only theoretical predictions but also detailed experimental data.
RIPL-4 will take advantage of this CRP to update the Gamma-ray strength function segment. It still needs to be decided if the information will be duplicated in RIPL-4 for specific files, or just provide a link to the Photon Strength Function website.
R. Capote and T. Kawano will assess if there is any specific issue related to actinides for fission cross section calculations.

### 5.7. Interfaces and retrieval tools (Coord: Capote)

Different options will be studied by IAEA (R. Capote) to update the interface and retrieval tools. Constraints from the cyber-security will have to be taken into account, especially when running codes in the background.

**Appendix I**

IAEA Atoms for Peace: The First Half Century 1957–2007

**1st Research Coordination Meeting on**

# "Recommended Input Parameter Library for Fission Cross Section Calculations (RIPL-4)"

IAEA Headquarters, Vienna, Austria
6 – 9 June 2017
Meeting Room MOE27

**Provisional AGENDA**

## Tuesday, 6 June

**08:30 – 09:30** **Registration** (IAEA Registration desk, Gate 1)

**09:30 – 10:00** **Opening Session**

Welcoming address and Introductory Remarks – Roberto Capote
Election of Chairman and Rapporteur
Adoption of Agenda

**10:00 – 13:00** **Presentations**

S. Goriely
S. Zhou
M. Kowal

***13:00 – 14:00*** ***Lunch***

**14:00 – 18:00** **Presentations**

S. Yavshits
N. Carjan
E. Grosse
E. Soukhovitskii

*Coffee breaks as needed*

## Wednesday, 7 June

**09:00 – 13:00** **Presentations**

M. Sin
T. Kawano
S. Hilaire
Han Y.

***13:00 – 14:00*** ***Lunch***

## Wednesday, 7 June (cont'd)

**14:00 – 16:00 Presentations**

O. Iwamoto
A. Koning

**16:00 – 18:00 Discussions on fission parameters to be provided and fission cross section calculations**

*Coffee breaks as needed*

## Thursday, 8 June

**09:00 – 13:00 Review of possible updates to additional RIPL Segments**

Masses (S. Goriely)
Levels (M. Verpelli)
Resonances (R. Capote)
Optical model segment (R. Capote)
Level density segment (S. Goriely)
Gamma-ray strength functions (E. Grosse)
Interfaces and retrieval tools

***13:00 – 14:00 Lunch***

**14:00 – 18:00 Discussions and drafting of the meeting report**

*Coffee breaks as needed*

***19:30 Dinner at a restaurant in the city***

## Friday, 9 June

**09:00 - 13:00 Drafting and review of the meeting report**

**13:00 Closing of the Meeting**

*Coffee break as needed*

First Research Coordination Meeting on

**"A Recommended Input Parameter Library for Fission Cross Section Calculations"**

IAEA, Vienna, Austria

**6-9 June 2017**

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