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SANDA Project D4.1: Report on code development and methods

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1. Introduction

This report summarizes the work performed in the work package 4 of the SANDA project. The efforts were targeting the support of evaluations, with theoretical and code developments. As one of the major step in the evaluation process is the production of nuclear data libraries, with eventually adjusted cross sections, nuclear reaction tools (TALYS, EMPIRE) should fulfil the user requirements regarding cross section quality, flexibility and format. The developments in this area are presented below. Additionally, open-source codes do not allow yet to perform calculations for all isotopes, especially in the range of light element. This represents a weakness for the development of a nuclear data library, and the current work package partially addresses this issue by supporting theoretical developments, which will eventually be incorporated in distributed codes. Examples are also presented in the following.

2. TALYS developments

TALYS is nuclear reaction code developed between the IAEA, the CEA DAM and the University of Brussels. It is freely distributed (with the source access) and is of benefits for the whole nuclear reaction community. It is continually improved, and SANDA, as well with its predecessors, has a significant impact on TALYS by allowing developers to get enough funding and time, in order to improve and update the code. Not only the nuclear energy community benefits from these developments, but also the accelerator community, as well as the medical isotope or the astrophysics communities. The SANDA efforts for TALYS are therefore of prime importance. The latest release is now available at both the IAEA Nuclear Data Section and the PSI TENDL websites.
Thanks to these new improvements of the code, the quality of nuclear data libraries is improving. This is true for the JEFF community (its latest release JEFF-3.3, and the current developments for the next release, JEFF-4), but also for the TENDL library (largely based on TALYS), and for ENDF/B-VIII.0, which import a number of JEFF and TENDL files. In the following, some details of the theoretical improvements and their applications (to evaluated nuclear data files) will be presented.

2.1. Improvements of models

In order to include the latest developments to improve the modelization of the inelastic cross sections for actinides, the full development of the Engelbrecht-Weindenmuller transformation was implemented in TALYS. It allows a proper treatment of direct reaction impact on compound nucleus reactions. It was validated and tested with U238 and Pu239 nuclear reaction models.
A non-negligible impact was found on both isotopes. All cross sections (radiative capture, fission, elastic/inelastic channels) were impacted from a few percent up to 10 percent for some channels (U238 inelastic first level reaction). An example is presented in Fig. 1 for the total inelastic cross section of ^{238}U.

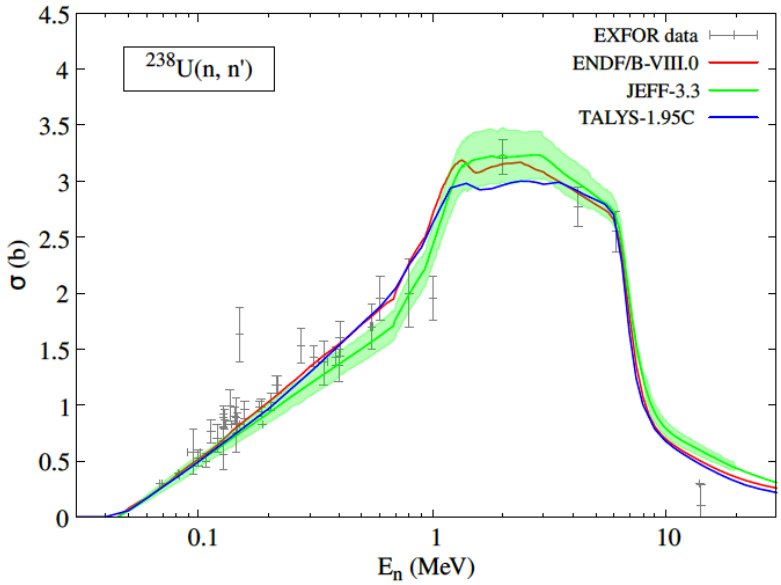

Figure 1. Example of the new modelization for the total inelastic cross sections of ^{238}U performed with the updated version of TALYS.

In parallel, the decay of fission products from TALYS was verified. J.F. Lemaitre developed a python code to drive TALYS and check externally the fission fragment decay implemented internally in TALYS. He managed to cross check results from the two ways of dealing with the same problem and found errors in the way the decay was implemented in TALYS. These errors have been corrected in TALYS and the results for the PFNS and nubar are much better now than they use to be. However, after a little bit more than one year, JF Lemaitre found a permanent position and could not conduct all the physical tests which were initially foreseen.

2.2. Nuclear reaction evalution

The future release of the JEFF library (in 2024) motivated the revision of the resonance range of the neutron cross sections of actinides (Pu239, U235, U238, U234, U236, Np237, Am241, Am243, Pu240, Pu242), fission products (Ag107, Ag109, Tc99, Xe135, Lu173, Lu175, Lu176, Pm148, Eu151, Eu153, Eu154, Eu155, Cs133, Cs135, La-139, Sm-151, Tm-171, Os-186,187,188) and structural materials (Mg-24,25,26, Fe-54,56,57).
The resonance analysis was performed with the nuclear data codes CONRAD and REFIT, which are developed at CEA/DES of Cadarache (France) and JRC-Geel (Belgium), respectively. The data sets introduced in the evaluation procedure come from the EXFOR database. The latest experimental results measured at the GELINA (JRC-Geel) and n_TOF (CERN) facilities were included in the resonance analysis. Results obtained for Pu239 and U235 were compared with the evaluations produced by Luiz Leal (IRSN) and Marco Pigni (ORNL) with the SAMMY code. This collaborative effort was managed by IAEA via the International Nuclear Data Evaluation Network (INDEN). An example of the resonance analysis obtained with CONRAD is presented in Fig.2.

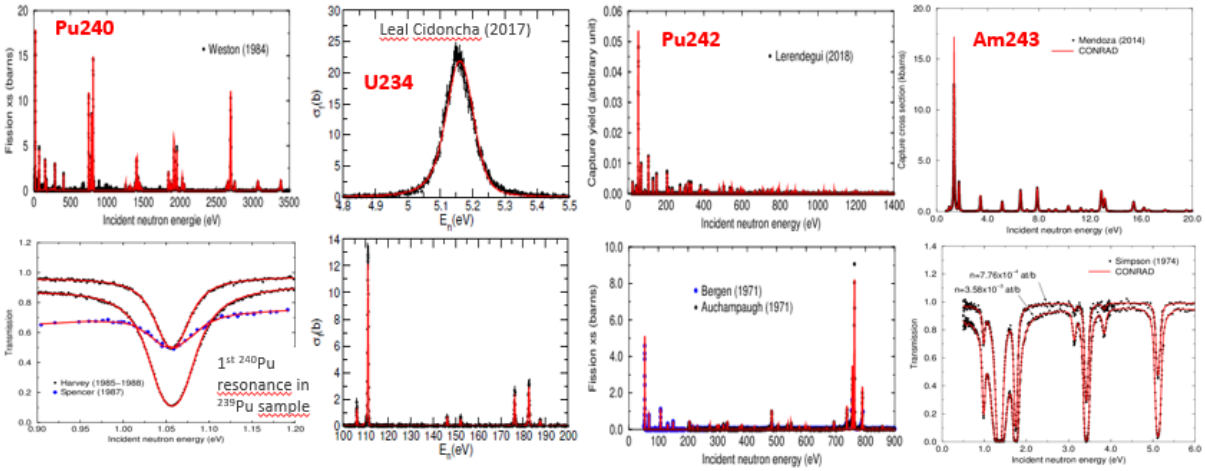

Figure 2. Examples of resonance analysis performed with the CONRAD code.

For some of the non-fissile isotopes, the resonance parameters reported in the literature were directly included in the evaluated nuclear data file. Emmeric Dupont (CEA/IrPhu Saclay, France) handled this work with the aim of including most of the resonance parameters delivered by the n_TOF community. Full evaluated nuclear data files for fission products were produced at PSI using the TENDL strategy. This strategy consisted of taking into account the resonance parameters recommended by evaluators. Negative resonances were slightly adjusted to reproduce the thermal cross sections compiled in the Atlas of Neutron Resonances. This approach is able to deliver consistent files in ENDF-6 with covariances.

2.3. New evaluations for JEFF and TENDL

As mentioned in the previous paragraphs, the TALYS developments, combined with the latest compilations of the resonance parameters from the n_TOF collaboration, has allowed to update a number of evaluations for important fission products. This is a combined efforts of all partners from the SANDA WP4. Such new evaluations consist of adjusted TALYS calculations in the fast neutron range, with new resonance parameters, all formatted in ENDF-6 files, to be included in nuclear data libraries. The main tool to produce such evaluations is the T6 system, and preliminary files are included in the latest release of the TENDL librara, TENDL-2023. It is freely available from the PSI TENDL website. In addition, after checking by the JEFF community, the same evaluated files are also included in the beta release of the JEFF-4 library. These new evaluations are also available for the whole JEFF community for testing. Such developments and improvements are only possible thanks to the SANDA funding, allowing better collaboration between groups which are located in different European countries.
Among the important fission products, it is worth mentioning new evaluations for ^{135}Xe, ^{133}Cs, ^{107}Ag, $^{151,153\text{-}155}$Eu, ^{173,175}Lu, ^{139}La, $^{186\text{-}188}$Os and ^{148m}Pm. An example of the changes in the resonance range for ^{107}Ag is presented in Fig.3.

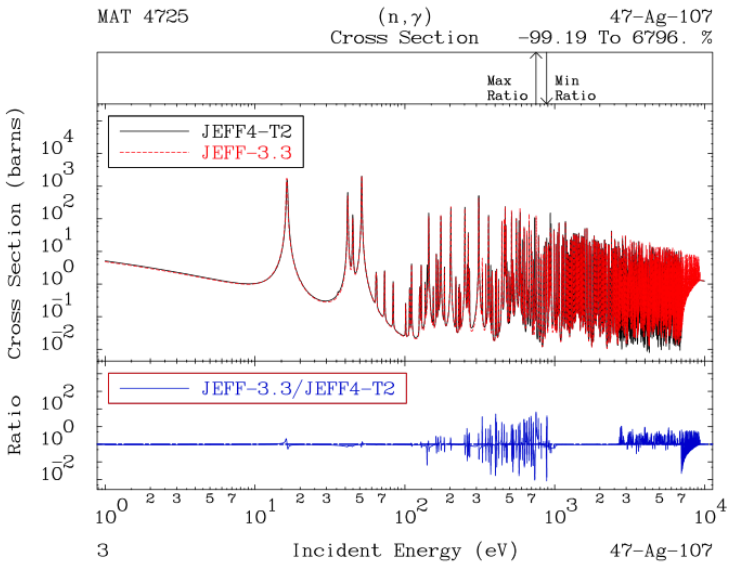

Figure 3. Example of the new resonance region for ^{107}Ag.

In addition, improvements were also realized for the minor actinides ^{236}U and its associated covariances. The current version of the JEFF-3.3 library does not contain covariance files for this isotope, and to remedy this deficiency, a collaborative effort between the CEA and PSI allowed to produce covariances based on the TMC approach. This new evaluation is proposed in the latest beta release of the JEFF-4 library. A last example of collaborative efforts between PSI, the JRC Geel and the CEA DES concerns the evaluation of ^{238}U and the adjustment of resonance parameters. It was noticed that the JEFF-3.3 and ENDF/B-VIII.0 libraries, which share the same resonance parameters for this isotope, produce reactivity swing for PWR calculations not in agreement with previous library releases. This problem was identified and linked to specific resonance parameters of ^{238}U. A modification of such parameters was performed at the JRC Geel and tested at PSI and the CEA DES, leading to an improvement of the k_{eff} calculations for PWR assemblies. Even if this issue is not fully solved, the current developments performed within SANDA clearly solved part of the discrepancies.

2.4. References

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3. EMPIRE developments

The work performed at the University of Bucharest (UB) focusses on performing nuclear data evaluation with the latest version of the reaction code EMPIRE. The IAEA evaluation of the neutron induced reactions on ^{239}Pu based on EMPIRE calculations in the 0.01-30 MeV energy range performed by UB within SANDA project was selected to be adopted by ENDF/B-VIII.0 (see Fig. 4). It is worth reminding that the evaluations for the other two major actinides $^{235, 238}$U based on EMPIRE calculations in the fast neutron region performed by UB within CHANDA project are already included in ENDF/B-VIII.0 and CIELO libraries.

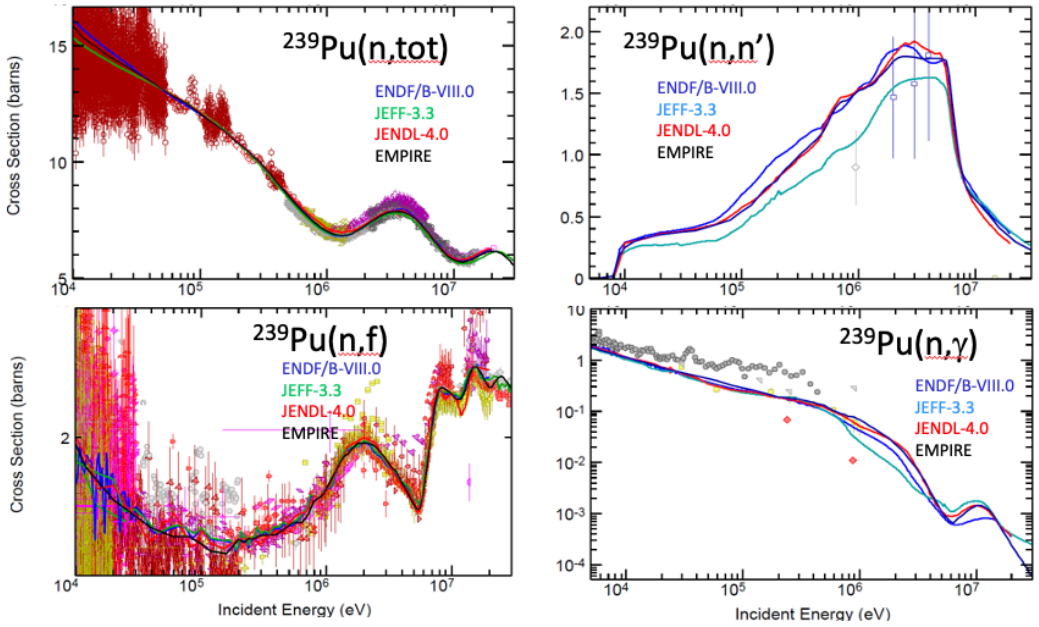

Figure 4. Model calculations for some n + ^{239}Pu cross sections performed with EMPIRE.

3.1. Availability of new EMPIRE modules and models

There are two aspects related to the availability of new EMPIRE modules/models: (A) the public access to the newest versions, which concerns mainly the users of this code, and (B) modules developed and tested in EMPIRE portable to other reaction codes, which are of interest for a larger part of the nuclear data community.

A. EMPIRE is a modular system of nuclear reaction codes using various theoretical models and represents a general, flexible, and easy to use tool for basic research and evaluation of nuclear data. Nuclear data evaluation is facilitated by the ENDF-6 formatting, file verification and graphical comparison with experimental data. EMPIRE code is distributed as a complete, self-contained and

install-free package. It is provided for the three most popular operating systems (Linux/Unix, Mac and MS Windows).

Maintaining, developing and updating the code to improve its evaluation capabilities for nuclear data and the associated uncertainties has been a permanent concern. Among the addressed issues we mention: dispersive optical potential with multi-band coupling, Moldauer width fluctuation correction, Engelbrecht-Weidenmuller transformation, compound nucleus anisotropy, level density formulation for equilibrium and saddle-points deformations, gamma strength functions, extended optical model for fission for multi-humped barriers with partial absorption in the wells, nubar, prompt fission spectra, the link with the resonance region, prior covariance matrices generation using either the Kalman filter or Monte Carlo sampling of the model parameters, etc. Some of these features became already publicly available, other are still under testing and validation.
EMPIRE-3.2.3 is the latest tested version which since November 2021 can be downloaded as portable version for MS-Windows 64-bit (including sources and installation scripts for 32-bit) or as sources and installation scripts for Linux and MacOS from https://www-nds.iaea.org/empire/index.html or https://www-nds.iaea.org/cdroms/.

B. Similar evaluations from different libraries show in many cases significant discrepancies. These can be explained using different codes, different models, approximations, implementations or different sets of experimental data considered in the evaluation process. To identify better the sources of discrepancies, an intercomparison of the main codes employed in evaluations (EMPIRE, TALYS, CCONE and CoH_3) using the same controlled set of input parameters was conducted. The results, presented at ND2016, proved to be very instructive. Therefore, within the IAEA CRP RIPL-4 it was suggested to continue the intercomparisons but making a step further: beside the same set of input parameters to use the same modules to calculate certain quantities such as level densities and fission transmission coefficients as being the largest sources of discrepancies. The EMPIRE code was considered the most appropriate to implement and test these modules.

Level density module. Most of the reaction codes are using for the level density description the Gilbert-Cameron formulation, the Generalized Superfluid Model or the microscopic HFB numerical tables, none of them being ideal for use on the entire excitation range of interest, especially in the case of deformed nuclei. It was agreed that the Constant Temperature (CT) part of the Gilbert-Cameron formulation works better at low excitation energies, while the Fermi Gas (FG) part of the Generalized Superfluid Model with collective enhancements and energy depending on damping factors performs better at higher excitation energies. A CT+FG model with parameters constrained to reproduce the cumulative numbers of low-lying levels and the average neutron resonance spacing at the separation energy has been recently implemented in EMPIRE and is ready for testing. A stand-alone version of the module easy to be implemented in other codes is also available.

Fission module. The fission module implemented in EMPIRE is well encapsulated, has separate input and output files and can be easily incorporated in other codes. It is based on the optical model for fission and proved to provide good descriptions of experimental fission cross sections from the simplest case of even-N compound nuclei populated in neutron induced reactions with double-humped fission barrier, up to the most complicated case encountered up to now which is photon induced fission on nuclei with triple-humped barriers. The parameters of the fundamental barrier can be retrieved from files extracted from RIPL containing the Maslov's empirical barriers and the microscopic HFB barriers, or from a custom library. The parameters of the barriers associated to the transition states are provided by the code based on RIPL recommendations. A problem represents the level densities at the saddle points, which is recommended to be described by the same model used for normal states. Presently, EMPIRE uses either GSM (adapted for the saddle points

deformations and asymmetries) or HFB. But, if for the normal states it is used CT+FG formulation mentioned before, then something similar has to be used for the transition states in continuum. Most likely, in this case only the CT part could be used for the entire range. However, without experimental information on cumulative levels and D_0, the parameters can be obtained only from an extensive fit of the available experimental cross sections, which requires time.

3.2. References

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4. Evaluation Techniques of Light Nuclear Systems (GECCCOS developments)

The work on subtask 4.1.1 at TU Wien focused on developments of evaluation techniques for light nuclear systems and their numerical implementations into GENEUS (GEneral Nuclear Evaluation Update System). The evaluation of reaction data of light nuclear systems requires a special process because of the lack of quantitatively reliable semi-classical models. Most evaluations of reaction data of light nuclear systems rely primarily on experimental data without reference to any a-priori information. In the absence of quantitatively reliable semi-microscopic models, one frequently performs phenomenological R-matrix analyses of experimental data. Albeit these analyses lead to excellent descriptions of reactions in light nuclear systems, they have no predictive power and are limited to binary channels and in energy. A complete unitary description of a nuclear system is not possible in general. However, the best R-matrix analysis does not substitute a nuclear data evaluation. At present there are still open problems how to perform a consistent Bayesian evaluation associated with R-matrix analyses. Within this subtask, the nuclear data group at TU Wien focused on these problems and developed an evaluation procedure based on R-matrix analyses of almost Bayesian nature. The proposed method was implemented in the module GENEUS-R which allowed detailed studies of the novel technique. The details of the work on subtask 4.1.1 performed at TU Wien are outlined in the subsections 4.1 and 4.2. In subsection 4.3 conclusions and an outlook of the work performed by the Nuclear Data Group at TU Wien are given.

4.1. Specifics of R-Matrix Analyses of Light Nuclear Systems

Light nuclear systems exhibit a scarcity of levels up to rather high excitation energies because of the small numbers of nuclei involved. The corresponding reactions in light nuclear system show resonant cross sections in this energy range. In general, microscopic nuclear models cannot provide a quantitatively accurate description of these cross sections. Therefore R-matrix analyses [Lane1958] are frequently used and yield excellent descriptions of resonances. Albeit non-microscopically based, R-matrix theory satisfies all conservation rules and provides a consistent set of reaction cross sections. However, R-matrix analyses of reaction data of light nuclear systems are not straightforward because of various reasons. (i) in several light nuclear systems, dominant breakup channels open at rather low energy and (ii) the application of R-matrix analyses is limited in energy for practical reasons because the number of open channels and therefore the number of parameters to be optimized is strongly increasing with energy. There exists no viable alternative because the application of the nuclear statistical model for light nuclei is questionable, especially in the transition region between resonances and intermediate energies. In order to provide solutions to these shortcomings of R-matrix analyses we proposed procedures to overcome these difficulties. In subsection 4.2 details of our developments and corresponding studies are briefly summarized

4.2. Towards a Bayesian Evaluation Technique for Light Nuclear Systems

The Bayesian evaluation of nuclear reaction data of medium heavy and heavy nuclear systems is well established. There exists a clear separation between experimental information and a-priori knowledge in terms of semi-microscopic models, where the latter provide quantitative reliable reaction calculations. An automatized process can be numerically realized to perform such Bayesian evaluations e.g. the code GANDR or the code GENEUS. The latter (GEneral Nuclear Evaluation Update System) is in development at TU Wien and provides an evaluation environment based on the modified GLS technique. The code also provides options for the inclusion of model defects via Gaussian processes.
The basis of the modified GLS technique is presented in [Schnab2017] and provides an efficient method for large scale evaluations. In this technique only a reduced covariance matrix of the dimension of the number of Monte Carlo sweeps MC is updated, i.e

$$\mathbf{W}_1 = \mathbf{W}_0 - \frac{1}{MC}\mathbf{W}_0\mathbf{V}^T\mathbf{X}\mathbf{V}\mathbf{W}_0 \quad \text{with} \quad \mathbf{W}_0 = 1 \quad \text{and} \quad \mathbf{X}^{-1} = \frac{1}{MC}\mathbf{V}\mathbf{W}_0\mathbf{V}^T + \mathbf{B}. \tag{4.1}$$

Key element of the algorithm is a matrix built of MC vectors of observables calculated by the model with randomly varied sets of parameters. The matrix, where mediates the transformation between model grid and the grid of experimental data and is the covariance matrix of experimental uncertainties. Using these expressions the Bayesian update of the mean value and the covariance matrix are simply given by

$$\vec{\sigma}_1 = \vec{\sigma}_0 + \frac{1}{MC}\mathbf{U}\mathbf{W}_0\mathbf{V}^T\mathbf{X}\left(\vec{\sigma}_{\text{exp}} - \mathbf{S}\vec{\sigma}_0\right) \quad \text{and} \quad \mathbf{A}_1 = \frac{1}{MC}\mathbf{U}\mathbf{W}_1\mathbf{U}^T. \tag{4.2}$$

The advantage of this formulation is the fact that only the matrices W_i must be stored which are usually of smaller dimension than the full covariance matrix A_i. Despite the smaller dimension W_i contains the full information for all covariance matrices for given channels.
At the beginning of the current project, we focussed on the inclusion of differential observables in order to enhance the completeness of the set of independent observables in GENEUS. In parallel we have put forward the evaluation of light nuclear systems and realized that there are several severe problems hampering a straightforward extension of the Bayesian technique to these systems. The major challenges are (1) the lack of a quantitatively reliable semi-microscopic theory. Therefore phenomenological R-matrix analyses of experimental data are usually performed which do not satisfy the conditions of an a-priori knowledge in Bayesian statistics. (2) R-matrix theory is limited to binary channels. Especially, dominant breakup channels may occur in light nuclear systems at rather low energy, which cannot be included in standard R-matrix theory. (3) In light nuclear systems resonant behaviour extends up to rather high energies (20 MeV and beyond) and a transition to a statistical nuclear model regime is questionable. An extension of R-matrix analyses to high energies is hardly manageable because of the significant increase of open parameters with increasing energy. Realizing these problems we focussed our work to tackle the challenges of nuclear data evaluations of light nuclear systems. In the following paragraphs the achieved developments are discussed in more detail.

Beyond standard R-matrix: Because of the limitation of standard R-matrix theory to binary channels a complete R-matrix analysis for light nuclear systems is almost impossible due to the occurrence of breakup channels. A possibility to surpass this problem was already discussed by Lane and Thomas [Lane1958] in 1958. They proposed the so-called Reduced R-matrix which explicitly includes only part of the channels, while the impact of the remaining ones is only globally taken into account. Although an exact expression for the Reduced R-matrix is given in their paper, we are not aware of any practical application except the frequently used Reich-Moore approximation [Reich1958]. Using a toy model we worked out a simplified expression for the Reduced R-matrix [Haisch2021] which yields fair results for well separated resonances and fully accounts for the thresholds of ignored channels. Independent from the present task the simplified expression was successfully applied in a Reduced R-matrix analysis of the n+9Be system up to incident neutron energies of 10 MeV. Especially, the dominant integral cross

section of the four-body breakup n+9Be → α + α +n+n with the Q-value at -1.665 MeV was well reproduced.
A further development, i.e. the extension of R-matrix analyses to higher energies, is important for nuclear data evaluations of light nuclear systems because a transition to mean fields approaches is questionable. Currently we are testing within R-matrix theory several phenomenological extensions to describe reaction cross sections at higher energies. The results are promising, but further investigations are still required for a final conclusion.

Proposal of quasi prior based on R-matrix calculations: R-matrix analyses are usually performed to describe reaction cross sections of light nuclear systems. In this process the R-matrix parameters are determined via optimization using available experimental data. Therefore an R-matrix analysis cannot represent the a-priori information. What is a-priori known is the level structure (energies and J□-values) of the compound nucleus system and the thresholds of different reactions. At low energies the pole-terms of the R-matrix analysis are frequently associated with the level of the compound nucleus, but usually at different energies depending e.g. on the value of the chosen matching radius. On the other hand the form and strength of resonances is related to the J^{π}-values. Taking these dependences into account we propose the following procedure to generate a prior associated with R-matrix analyses. First we perform a Reduced R-matrix analysis of the considered system and determine via the criterion of Turchin [Turchin1970] the acceptable variations of the pole terms and the reduced width parameters. For the pole terms we also consider the distance to the associated level of the compound nucleus. Then we initiate a Monte Carlo procedure with R-matrix calculations randomly varying (uniform distributions assumed) the pole terms, the reduced width parameters and the matching radius. Performing MC~200-500 Monte Carlo sweeps we can determine a full covariance matrix for all channels which contains the essential features of the R-matrix, but least information of the R-matrix analysis itself. Essentially, only the information about the resonance form enters via the covariance matrix $\mathbf{A_0}$. Thus the associated vector $\vec{\sigma}_0$ of mean values and the covariance matrix $\mathbf{A_0}$ include characteristic features of R-matrix theory but only minimal information from experimental data. Therefore it appears justified to consider ($\vec{\sigma}_0$, $\mathbf{A_0}$) as an applicable prior for a Bayesian evaluation. As an example we used the available Reduced R-matrix analysis of the n+^{9}Be system and generated the prior as discussed above. The mean values and their error bands for some channels are shown in Fig. 5. These results do not show the structure of the original experimental data. Nevertheless, $\mathbf{A_0}$ contains important information about the form of resonances in R-matrix analyses.

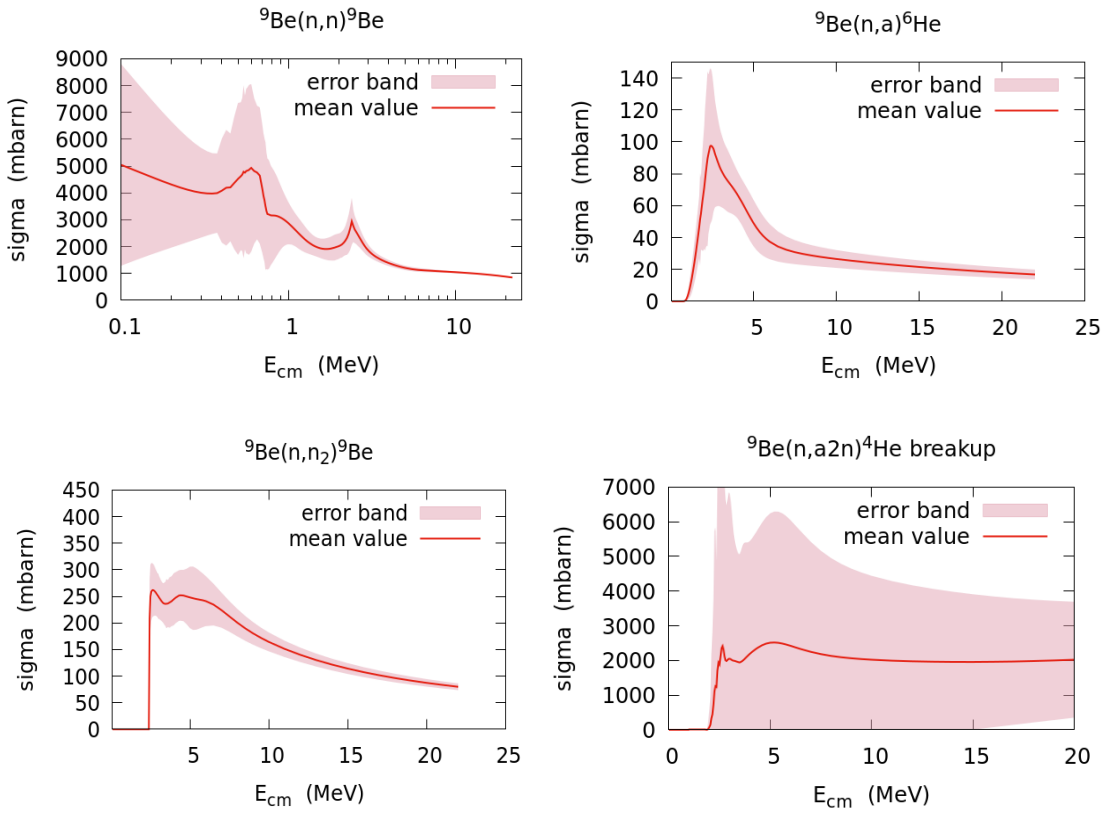

Figure 5. Mean values and error bands (2σ) of the prior for reactions in the n+^{9}Be system.

Bayesian evaluation for light nuclear systems: Generating the prior as discussed before the Bayesian evaluation can proceed as discussed e.g. by Schnabel and Leeb [Schnab2017]. We constructed a module GENEUS-R, which allowed us to generate the prior as discussed above and perform a Bayesian update procedure via the modified GLS-method. The module includes an extended part which reads experimental data files and generates covariance matrices **B** including statistical and correlated uncertainties of the experiments. The correlated errors are assume with 3% for the elastic channel, 5% for the inelastic and the (n,α) channels and 1% for the total cross section. Correlations between experiments are not taken into account. In this first version of GENEUS-R we restricted ourselves to angle integrated data. Similarly to before we used the available Reduced R-matrix analysis of the n+^{9}Be system up to 10 MeV neutron energy and performed the update procedure as described above. In Fig. 6 the final results of the Bayesian evaluation are displayed. The error bands are in the order of 1-2%.

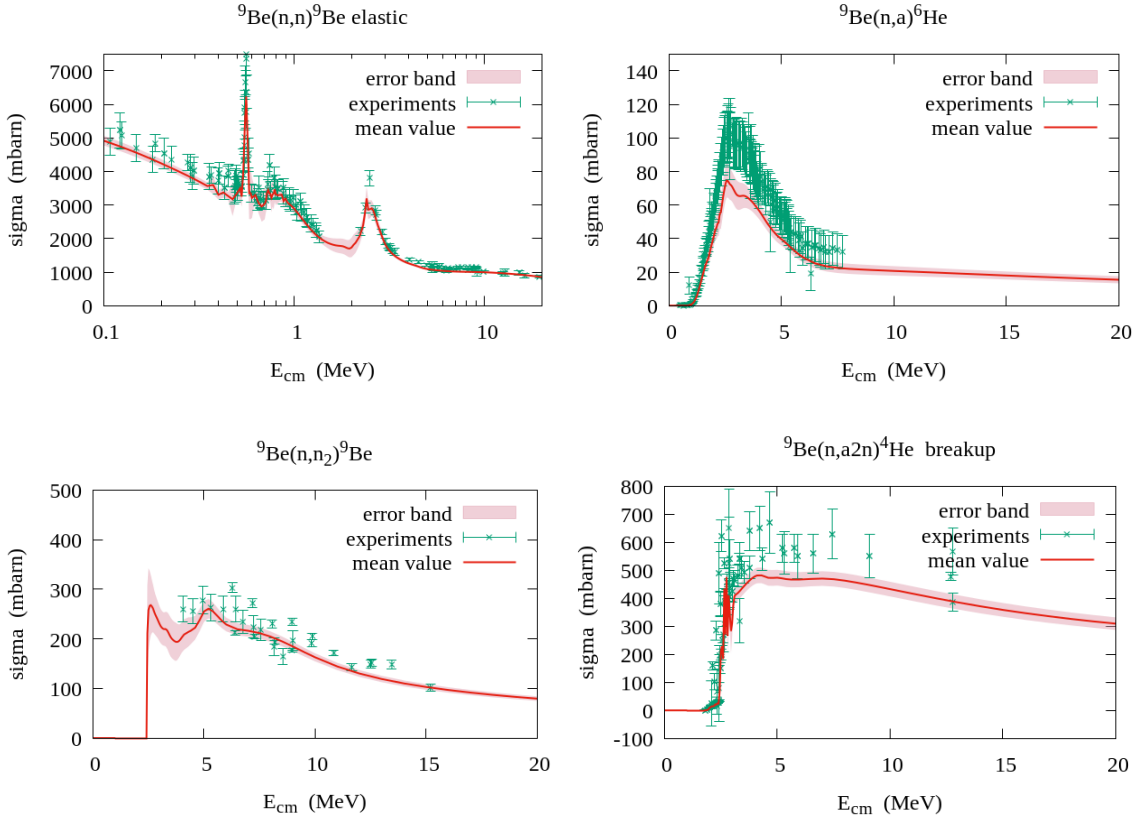

Figure 6. Various cross sections for reactions in the n+^{9}Be system.

The Bayesian update via the module GENEUS-R also provides covariance matrices of the uncertainties. It is the peculiar feature of the modified GLS-method that not the full covariance matrix must be stored because the whole information is included in the matrix W_1, which is of smaller dimension. Using an adapted version of Eq. (4.2) allows the determination of channel covariance matrices of interest. Examples for some reactions and cross correlations between reactions are shown in Fig. 7.

The Bayesian update procedure provides an excellent description of neutron-induced reactions up to 10 MeV and is subject of a paper in preparation [Leeb2023]. It is remarkable that even the breakup channel, although not explicitly considered, is well reproduced. The covariance matrices of the reaction channels do not show significant structures. The diagonal elements of the correlation matrices of one reaction channel are all Corr(i,i)=1.0, but the diagonal is not completely seen in the figures because of the strong decrease off the diagonal.

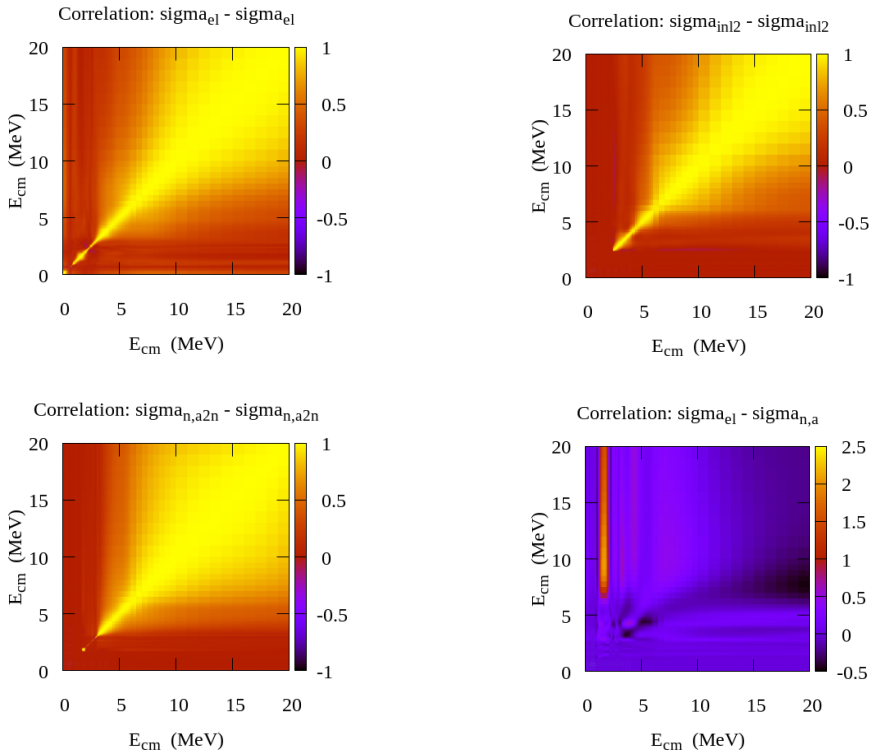

Figure 7. Correlation matrices for different channels and cross correlations between different reaction channels in the n+^{9}Be system.

4.3. Summary and Outlook

The central goal of the Nuclear Data Group at TU Wien within the subtask 4.1.1 of the present project was the development of a Bayesian evaluation technique for light nuclear systems. In the course of the work we succeeded to generate a prior which represents a-priori information and includes the basic features of R-matrix analyses, while the impact of available experimental data is kept minimal. On the basis of this prior a Bayesian evaluation update could be formulated and numerically implemented in a module GENEUS-R which is based on the modified GLS-technique worked out previously. Using an available Reduced R-matrix analysis of neutron-induced reaction data of ^{9}Be we could successfully demonstrate the feasibility of the proposed algorithm. The evaluated results excellently reproduce available experimental data up to 10 MeV even for the breakup-channel. However, beyond 10 MeV available experimental data of other channels are not included in the present calculation. Thus the values of the breakup channel also include the contributions from these not considered channels.
The inclusion of channels opening at energies beyond 10 MeV requires an extension of the R-matrix concept to higher energies. Currently we are testing various proposals for a phenomenological extension of the R-matrix to higher energies. First applications are very promising but still require further studies. The presented analysis leads to rather small uncertainties especially for the elastic channel. This observation is similar to the results of other evaluations, which assume that the included models are perfect. As shown in previous studies of our group the inclusion of model defects may cure this problem. However, their formulation for the resonance regime is not straightforward. Raab et al. [Raab2019] presented a first formulation of model errors in the resonance regime. However, the suitability of this approach requires still studies with actual experimental data. Studies in this direction are currently in progress in the Nuclear Data Group at TU Wien.

4.4. References

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5. Uppsala developments

The overall aim of the subproject is to continue developing methods for TALYS based evaluation using an evaluation pipeline [Schnabel21], develop techniques for treating model defects, and account for unknown sources of uncertainties in experimental data. Below, the contribution during the reporting period is summarized. To that aim, the researcher Alf Göök was hired to contribute to the project.

5.1. Upgrade to run on HPC cluster

A TALYS calculation typically take seconds to minutes to predict relevant cross sections on the calculation energy grid. Even though the time consumption for a single calculation is moderate, hundreds to thousands of model calculations are needed during a full evaluation. The parallel execution of nuclear model calculations on a multi-processor machine or computer cluster is therefore a necessity. Even on a powerful multi-processor machine the full execution of the pipeline can take days to complete for each nuclide. For this reason, an effort has been made to enable the execution of the pipeline on high-performance computing (HPC) clusters. With the overall aim of a pipeline that creates fully reproducible nuclear data evaluations the pipeline is containerized, so that it can be used independently of the operating system and hardware platform. The original prototype pipeline used the container platform Docker [Schnabel2021]. However, due to security issues, Docker is not allowed on most high-performance computing (HPC) clusters. Therefore, the pipeline has been moved to the Apptainer/Singularity platform. Apptainer, being the open-source version of Singularity, is designed for ease-of-use on shared systems and in HPC environments. In the new implementation, the container can run entirely on the cluster that also performs the computationally expensive model calculations. A new package that wraps and runs the Talys calculations via message passage interface (MPI) has been written. The new implementation has been tested on Uppsala University's resource for high-performance computing UPPMAX. The full execution of the Cr-52 evaluation uses about 500 corehours of computing resources and could be executed within less than 5 hours on UPPMAX's Rackham cluster using 100 cores for parallel execution.

5.2. Update of TALYS prediction mapping to EXFOR observables

Nuclear model codes, such as TALYS, are capable of predicting a large variety of observables. TALYS writes its predictions in the form of ASCII formatted numeric tables to files. The availability of

predictions for all measured quantities is essential in evaluations where a nuclear model is employed as fitting function. For the prototype pipeline the R-package talysExforMapping was developed in order to enable evaluations with as large amount of experimental data extracted from the EXFOR library as possible. The vision is to eventually be able to account for all available and trustworthy experimental data in the EXFOR library. We have been extending this package in order to include a larger number of observables present in the EXFOR database. An updated version of talysExforMapping now allows the mapping between talys prediction and EXFOR observables on all total and residual production cross sections, in addition to total, elastic and inelastic scattering and exclusive cross sections.

5.3. Parallelization of the Levenberg-Marquadt Algorithm

The Levenberg-Marquadt (LM) algorithm is used in the pipeline to locate the parameter vector associated with the maximum a posteriori probability (MAP). The LM algorithm is a natural extension of the generalized least square method to a non-linear model. Because the LM algorithm is iterative it is typically computationally costly, and we have continued to study the efficacy of using this approach in the project. Hence, we have been researching methods for decreasing the computational cost of the LM algorithm. This effort includes implementing Broydens rank-1 update of the Jacobian [Broyden1965] instead of recalculating the full Jacobian in every iteration. However, the results of using Broydens rank-1 were inconclusive, and no recommendations can be made. Aside from the calculation of the Jacobian, the LM algorithm is inherently sequential. This is because the step length in parameter space for the next iteration is determined by comparing the expected to the real gain in likelihood of the former iteration. However, a parallelized version can be made by simultaneously trying several step lengths in each iteration. If the number of step lengths tried is smaller or equal to the number of available processors, this does not increase the computation time but optimizes the step length in each iteration. Thereby, the number of iterations needed to reach the MAP is reduced. This strategy has been implemented in the pipeline. It reduced the number of iterations to reach the MAP when applied to the Fe-56 case by about a factor of two. Since the model has several hundred free parameters that need to be varied in each iteration to compute the Jacobian matrix, the number of model invocations are significantly reduced.

5.4. Model defects

Nuclear models are often if not most of the times deficient. By deficient we mean that the model cannot reproduce the true cross-section, no matter its input parameters. To not bias the result of a model fit and to account for the model deficiencies in the uncertainty quantification, they must be treated. In the pipeline we account for model deficiencies in two ways, by letting the model parameters vary smoothly with the incident neutron energy, and to explicitly model the discrepancy between model and experimental data using a Gaussian Process (GP) in the observable domain. The smoothly varying model parameter treatment is based on ideas proposed and explored in [Helgesson2018] to use the capability of TALYS to allow variations of parameters as function of incident energy to simulate the treatment of model defects. We have extended the approach by introducing other covariance functions, in particular to allow for faster variation of the model parameters at low energies while keeping the variation smooth at higher energies.

It has been observed that the variation in the energy-dependent parameters is potentially too strong in comparison with the magnitude of the uncertainties. The uncertainties do not appear to be conservative and relatively small in some regions. This is believed to be caused by residual model defects that could not be treated by the energy-dependent parameters. For this reason, the treatment of model defects in the pipeline has been extended to also include a term in the observable domain. That is, we model the data vector y as

$$y_i = f(E; \beta(E)) + \varepsilon_m + \varepsilon$$

where ε is the experiment uncertainty, $\beta(E)$ is the energy dependent parameter vector and an additional model defect term ε_m is added. The defect term is represented by a Gaussian process centered at zero, with a squared exponential covariance function. The hyperparameters of the GP's covariance function is determined using marginalized likelihood optimization (MLO). The MLO is performed using a linearized TALYS model around the parameter vector found by the LM algorithm before including the ε_m term. To avoid the momentous bookkeeping that arises due to cross section sum rules, ε_m is not added to the evaluated TALYS model but only retained in the covariance structure used in the LM algorithm and in the posterior parameter covariance. A linearly interpolated GP has been used to reduce the computational cost of using GPs in the observable domain. A linearly interpolated GP is similar to a sparse GP. The presentation of results of this procedure is beyond the scope of this report but appears promising. In particular, strong spikes observed in the energy-dependent parameters are reduced. Furthermore, the resulting chi-square of channels not affected by resonance structure is improved on the expense of channels affected by the resonance structures.

5.5. Parameter transformation and construction of a prior

Most of the parameters in TALYS have little or no impact on the cross sections, measured by experiments, that are considered in the evaluation. However, there is knowledge on how uncertain the parameters are from other nuclides; certain restrictions on the parameters may even be considered part of the models themselves. Therefore, there is reason to assume a prior distribution for the model parameters. In the pipeline we use a multivariate normal distribution (MVN) for this purpose. In addition to the prior uncertainties, the parameters are constrained to values that TALYS accepts. The support of the MVN must be limited to the parameter values that TALYS accepts. Therefore, we use a transformation

$$p_{int} = p_0 + \Delta\, erf\left(\frac{p_{int} - p_0}{\sqrt{2}\Delta}\right)$$

This gives two parameter domains, an internal domain p_{int} where the parameter values can take on any real value, and an external domain p_{ext}, which is seen by TALYS. In the external domain the parameter values are constrained to the interval $(p_0-\Delta, p_0+\Delta)$, where p_0 is the prior expectation value, and Δ is taken as the distance to the closest parameter bound defined by TALYS. An MVN-prior is defined on the internal parameter domain. The prior uncertainty is assumed to be a multiple of the parameter uncertainty σ_0 published in [Koning2012], i.e. $\sigma = M\,\sigma_0$, currently M=2 is chosen. To avoid bimodal parameter distributions in the external domain a maximum prior uncertainty must be imposed. This results in the condition $\sigma \leq \Delta$; for a normal distribution in the internal parameter domain with $\sigma = \Delta$, a uniform distribution on the interval $(p_0-\Delta, p_0+\Delta)$ is obtained in the external parameter domain. In Fig. 8 examples of parameter values in the internal and external parameter domains, sampled from the posterior distribution, are shown.

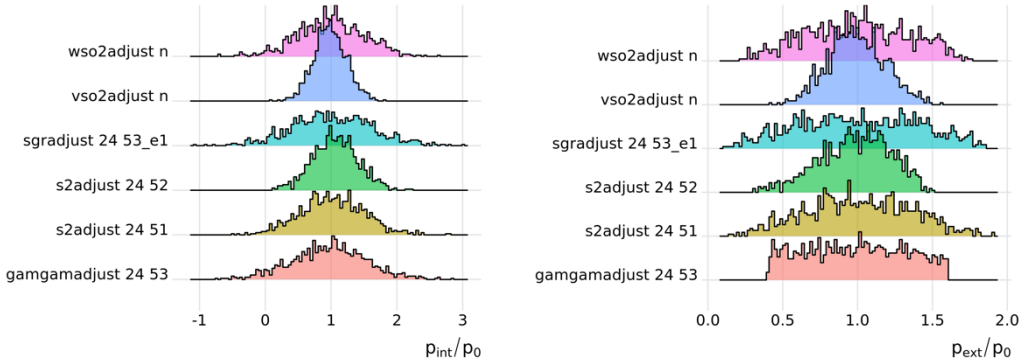

Figure 8. Example of parameter values sampled from the posterior probability distribution in the internal and external parameter domains.

The parameter transformation, as well as the prior uncertainty, differs from what was implemented in the original prototype pipeline, in which all parameters where limited to the same range and the same uncertainty of 10% was assumed for each parameter. For a number of parameters the assumed 10% uncertainty was significantly smaller than those estimated in [Koning2012], this could lead to an underestimation of the uncertainty in the evaluated cross-sections. However, increasing the parameter uncertainty without modifying the parameter transformation leads to unrealistic distributions. A larger uncertainty than allowed for by the transformation results in a u-shaped bimodal distribution of parameter values in the external domain, with the probability mass concentrated around the edges of the interval allowed by the transformation.

5.6. Minor updates and bug-fixing

In addition to the above-mentioned pipeline updates, several minor updates have been performed, such as new rules on how to determine the hyper-parameters of the GP and new techniques for updating the parameter values for parameters insensitive to experimental data. In addition, systematic testing and bug-fixing of the pipeline have been performed. We have also started to work on generalizing the script pipeline to be able to automize the evaluation for different nuclides. An example posterior distribution of ^{52}Cr cross sections is seen in Fig. 9.

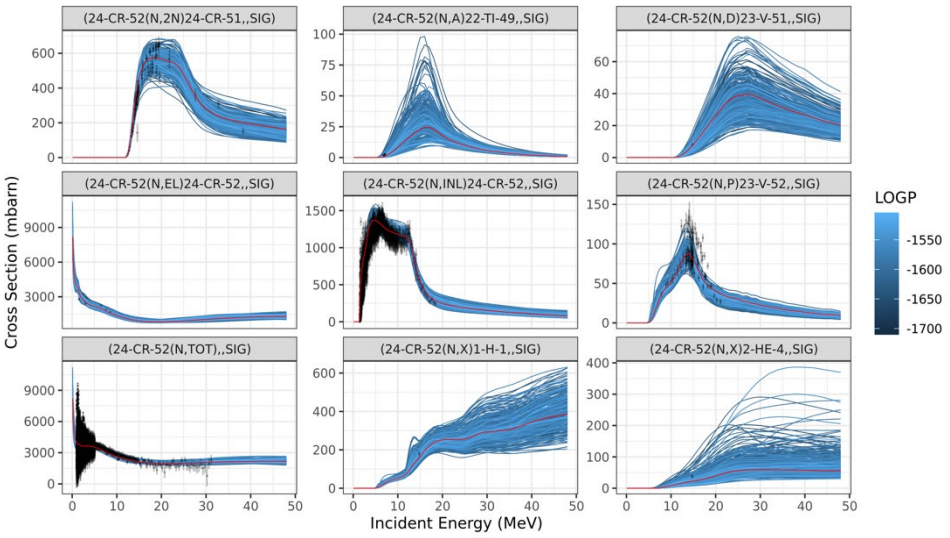

Figure 9. Cross section curves corresponding to random samples from the posterior probability distribution of parameters compared to experimental data. Each curve corresponds to one sampled parameter vector

and is color coded according to the posterior probability of that sample. The red line shows the cross section corresponding to the MAP found by the LM algorithm.

5.7. Conclusion

We are developing an evaluation pipeline encompassing all stages of the nuclear data evaluation process, from retrieving experimental data and preparing it to fit a nuclear model and generating ENDF files. We are aiming at a modular design, where an evaluation can be performed at the push of a button, to enable rapid testing of new algorithms and modified assumptions. In the present sub-project we have focused on the development of ways to treat nuclear model deficiencies, which can have a significant impact on the accuracy and reliability of evaluations. We inject more flexibility in the nuclear model using energy dependent parameters controlled by Gaussian processes. We also treat model deficiencies by inflating the experimental uncertainties, using Gaussian Processes in the observable domain. We have also focused on the further development of information technology tools to speed up the execution of the pipeline and to support the execution on high-performance computing clusters, a prerequisite for the automation of the evaluation process using computationally expensive nuclear models.

5.8. References

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6. Summary and conclusions

The collaborative efforts for the improvements of reaction codes and evaluations, performed within the WP4 of the SANDA project, have provided a number of improvements for the whole nuclear reaction community. This concerns naturally the main reaction codes EMPIRE and TALYS (freely available), the evaluation system in the light nucleus range GECCCOS, the evaluation system CONRAD, as well as the new evaluation procedure as developed at the Uppsala University. Evaluated data files were also produced within this project, with a clear benefit for the major nuclear data libraries and their users: better fission products and actinides representations.

Such developments, codes but also evaluated nuclear data files, are now available without restrictions through different websites (IAEA, PSI and NEA). But the main gain provided by the SANDA project is to allow the continuous efforts performed through decades of European collaboration, within some challenging periods of times with the COVID pandemic, the decrease of the number of evaluators and global funding for nuclear energy applications. We are nevertheless presently in a good position to abord the future of the nuclear renaissance thanks to the SANDA support. The evaluation and code developer community is currently very active, producing high quality evaluations, reaction codes and novel methods, naturally thanks to national programs, but also thanks to the EU SANDA project and European work.