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EMPIRE's ultimate expansion: resonances and covariances

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Abstract. Developement of the nuclear reaction code system EMPIRE since the last Nuclear Data Conference in Santa Fe (2004) is summarized. We report on the recent use of the code for the ENDF/B-VII.0 evaluations and concentrate on the two major directions in which the code is being expanded - resonances and covariances. Finally, we discuss exciting perspectives offered by parallel supercomputing.

1 Introduction

EMPIRE [1] is a complex system of codes, linked through a series of scripts and graphical interfaces, designed for modeling nuclear reactions. The system is general and flexible, and can been applied to the calculation of neutron capture in the keV region, as well as for the research of Heavy Ion induced reactions at several hundreds of MeV. Such broad range of incident energies and projectiles is possible thanks to the extensive set of nuclear reaction models that includes all nuclear reaction mechanisms that are important below 200 MeV. Comprehensive library of input parameters and graphic user interface facilitate preparation of the input and operation of the code. The major emphasis is on nuclear data evaluation and large part of the system is dedicated to ENDF-6 formating, checking, plotting, and processing through the NJOY code. This way, EMPIRE covers the complete evaluation cycle up to the preparation of files for transport calculations with the MCNP code.

Over the recent years, the system has been continuously extended and improved to meet evaluation exigencies posed by the development of ENDF/B-VII.0 [2]. We only give a very brief summary of recent changes and elaborate a bit more on ENDF/B-VII.0 and two new fields of expansion: neutron resonances and cross section covariances.

2 Recent developments

- **Automatic fitting of optical potential parameters** has been introduced in addition to the manual version present in the previous release. The fitting is highly automatized - user must only select parameters to be varied and EMPIRE extracts useful experimental data from the EXFOR library, sets suitable incident energy grid and performs minimization. Fitting is performed using Coupled-Channels model with the same coupling scheme, the same models and the same parameters as those used in the actual calculations. The procedure is stable (conservative) i.e., if no clear improvement is found EMPIRE retains initial parameters rather than pushing them to unphysical values.
- **Full support for dispersive Coupled-Channels optical potentials** has been introduced. This modification consits in allowing different geometry for the real and the imaginary volume potentials. This change enables EMPIRE to utilize physically sound class of optical model potentials that proved to provide excellent results with fewer parameters.
- **DWBA calculations to discrete levels embedded in the continuum** is a trick to increase high energy part of the neutron spectra. It compensates for shortcomings of the reaction models that in certain cases are unable to properly account for the collectivity of highly excited states.
- **DWBA calculations on odd targets** have been incorporated to enable use of the direct reaction mechanism when Coupled-Channels potential is not available or there is a necessity of using direct mechanism for the levels that can not be included within the Coupled-Channels coupling scheme. Since DWBA calculations can not be performed on targets with non-integer spins actual computations are done for a neighboring nucleus with even number of nucleons.
- **Deformed Multistep Direct model** is an extension of the original TUL approach to account for the effect of nuclear deformation on the RPA response functions. The modified model successfully reproduced spectra of inelastically scattered neutrons on ^{232}Th [4].
- **Improvement of the fission channel** has been continuous. Already sophisticated fission model that has been used for ENDF/B-VII.0 evaluations (see fig. 1) has been refined. Current advances include absorption in the third well, more general shapes of the fission barriers including those obtained in the microscopic Hartree-Fock-Bolgolyubov

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(HFB) calculations as well as level densities derived combinatorially from the HFB single-particle levels [6, 7].

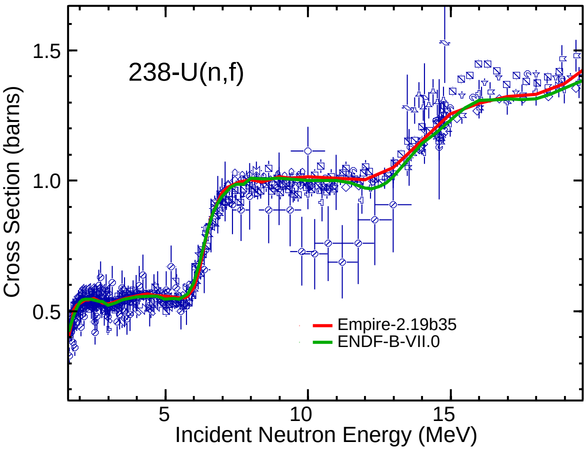

Fig. 1. Comparison of EMPIRE calculations with ENDF/B-VII.0 cross sections for ^{238}U(n,f) demonstrating how well calculations can match recommended values for this top priority reaction.

– **Improvements in ENDF-6 formatting and plotting** were introduced while developing the ENDF/B-VII.0 library. Here we mention only a mixed representation for storing spectra in the ENDF-6 format. This procedure separates reaction channels into exclusive and inclusive and stores the respective spectra in one of the two formats throughout the whole energy range.
– **Prompt fission neutron spectra and nu-bars** are important additions that make evaluated files for actinides complete. They are calculated including post-fission neutrons emitted from fully accelerated fragments and pre-fission neutrons. Both, nu-bar and PFNS calculations are consistent with the calculated fission cross sections.

3 ENDF/B-VII.0 evaluations

Development of the ENDF/B-VII.0 was an occasion for a first large scale deployment of the EMPIRE code. It has been used for 74 out of 393 neutron evaluations contained in the library. In most cases these are completely new files up to 20 MeV, in which fast neutron range and sometimes also unresolved resonance range are fully based on the EMPIRE calculations. The basic role of the experimental data was to determine model parameters. In some cases minor adjustments were imposed on the calculated results in order to match high quality experimental data. Contrary to a common practice, such adjustments were carried out during the calculations so that they were consistently propagated onto all reaction channels.

The EMPIRE based evaluations are complete: they include all reaction channels of importance for neutronics calculations, angular distributions, double-differential spectra, and recoils. The photon production spectra are provided for all reaction channels involving emission of γ-rays. The results were obtained using up to date reaction theory including Coupled-Channels and DWBA models in the incident channel and inelastic scattering, quantum-mechanical preequilibrium emission of neutrons (Multistep Direct and Multistep Compound), exciton model for emission of protons, α-particles (the latter with Iwamoto-Harada extension) and photons, widths fluctuation correction at incident energies below 3 MeV and sequential emission Hauser-Feshbach with full γ-cascade. For the materials of high priority the optical model parameters were adjusted in the course of evaluation. In general, we preferred to perform evaluation for the whole chain of isotopes since this allows for a more reliable constrain of model parameters and ensures consistency between the isotopes. In fig. 2 we show, as an example, capture cross sections for the extensive set of gadolinium isotopes.

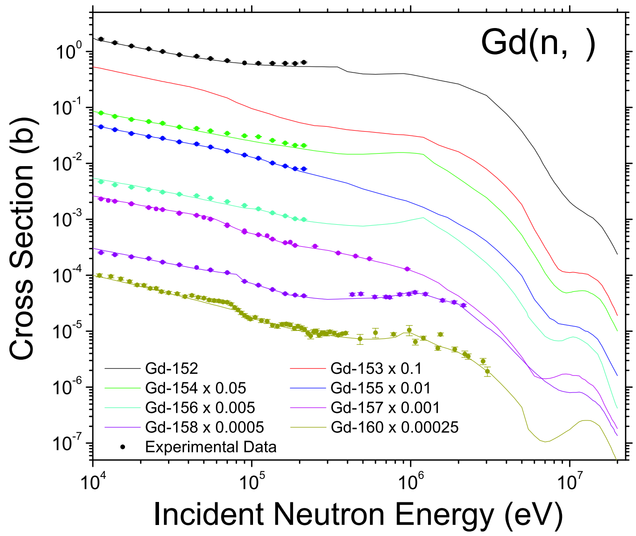

Fig. 2. Capture cross sections for Gd isotopes compared to experimental data in the fast neutron region. The neighboring curves and data are scaled by factors indicated in the legend.

4 Resonance module

EMPIRE-2.19 has been using an internal, ENDF-6 formatted, database of resonances to complete fast neutron evaluations with the resonance region. Recently, Mughabghab completed his Atlas of Neutron Resonances [3], a monumental compilation/evaluation work across the whole table of isotopes. This wealth of information must find its way into the evaluated libraries. With this goal in mind, we have started a new EMPIRE module [5] that will provide easy access to the Atlas data and their seemless transfer to the evaluation. We also intend to preserve legacy codes and methodology that has been developed over years and constitutes scientific heritage of great importance for application of nuclear technology. We stress, that the new module is intended for extracting and further processing of resonance parameters and properties collected in Atlas, i.e., it is not replacing codes used to analyze experimental data such as SAMMY or REFIT.

Contents of the Atlas includes actual resonance parameters (energies and widths along with uncertainties) and resonance properties (thermal cross sections, scattering radius, average resonance spacings, and average radiative, neutron and fission widths for s-, p-, and d-waves). The task of extracting, analyzing and formating of these quantities is delegated to the codes PTANAL and WRIURR that run in sequence supported by a few utility codes.

PTANAL assigns orbital momentum and spins to resonances if such were not determined form measurements. When doing it PTANAL makes use of the Bayesian method and random assignment respectively. In addition, average radiation width is calculated and assigned to the resonances with unknown radiative width and the fitting of reduced neutron widths to the Porter-Thomas distribution is performed. The completed set of resonances is stored in the ENDF-6 format (File 2) and passed to the WRIURR code along with the average resonance parameters. WRIURR constructs the unresolved resonance region using average parameters and appends it to the ENDF file.

RECENT, LINEAR and SIGMA1 codes are used to reconstruct pointwise cross sections for plotting against experimental data retrieved automatically from the EXFOR library. Graphic user interface (GUI) will allow the evaluator to adjust boundaries of resolved and unresolved resonance regions, the average resonance parameters and their energy dependencies in order to reproduce measured cross sections. The concept GUI for the resonance module is shown in fig. 3. Merging of the resonance region with the fast-neutron part of the evaluation will be performed with the existing code ENDRES.

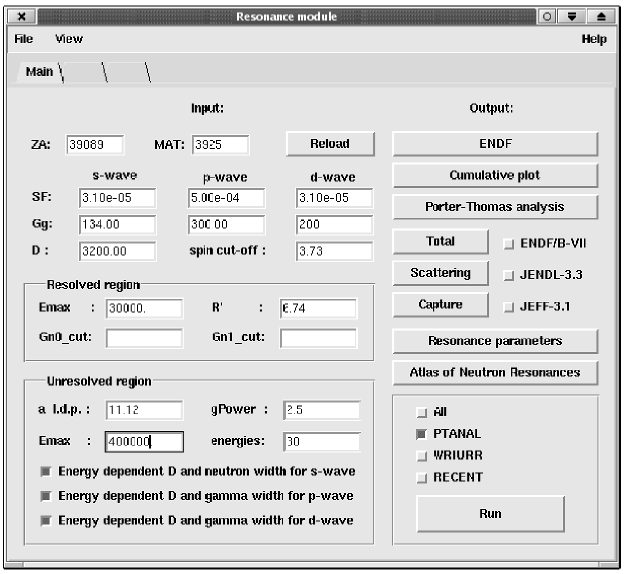

Fig. 3. Conceptual design of the future graphic user interface controlling the resonance module of EMPIRE. Average resonance parameters are retrieved form the Atlas and can be adjusted by the evaluator. Statistical analyzes of the resolved resonances (cumulative plots and Porter-Thomas analysis) are accessible through a click of a button as is also the graphical comparison of reconstructed cross sections with experimental data and other evaluations.

5 Covariance module

The methodology for generating cross section covariances in the fast neutron range was developed recently by the National Nuclear Data Center (BNL) in collaboration with the T-16 group (LANL). It employs a sensitivity matrix produced with the code EMPIRE, and uses it in the KALMAN code for determining covariances while taking into account relevant experimental data.

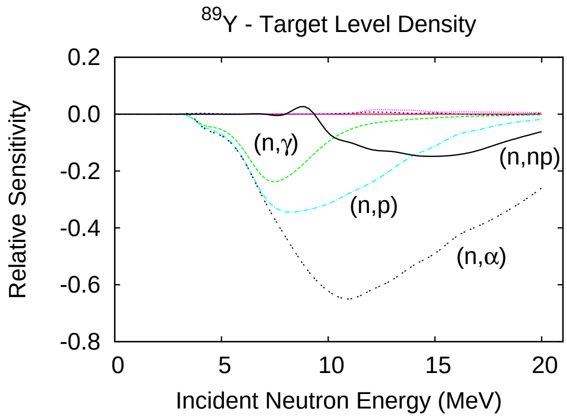

Fig. 4. Relative sensitivity of various reaction channels to the perturbation of the level density parameter in the target nucleus (^{89}Y) by 10%.

To obtain the sensitivity matrix, the most relevant model parameters in EMPIRE (optical model, level density and preequilibrium strength) are varied independently around the optimal value, to determine their effect on cross sections (see figs. 4 and 5). Sensitivity matrix elements are calculated as a change of a given reaction cross sections in response to the change of a particular model parameter. A series of scripts is employed to transfer such sensitivity matrix information along with the experimental data to the KALMAN code, and to prepare adequate input.

Fig. 6 shows an example of the correlation matrix. We note, that final uncertainties are adjusted to reproduce error bars on the best measurements by preventing errors on model parameters (initially set at 10 %) from falling below reasonable limits (3 %). This procedure is necessary since the Kalman filter tends to reduce uncertainties on model parameters if many consistent experimental data are well reproduced by the model calculations. The sensitivity matrices turn out to be very valuable off-spin of the covariance calculations. They allow for a deeper insight into the reaction mechanism, and offer extremally useful guidance in adjusting model parameters. Full set of sensitivity plots allows to determine which parameters should be changed in order to achieve required change in the cross section. At the same time the effect of the change on other reaction channel can be predicted and collateral damage minimized. Figs. 4 and 5 show that the effect of variation of some of the parameters reveal marked and difficult to anticipate energy dependence. Therefore, combined adjustment of several parameters might be very effective in reproducing experimental data with theory.

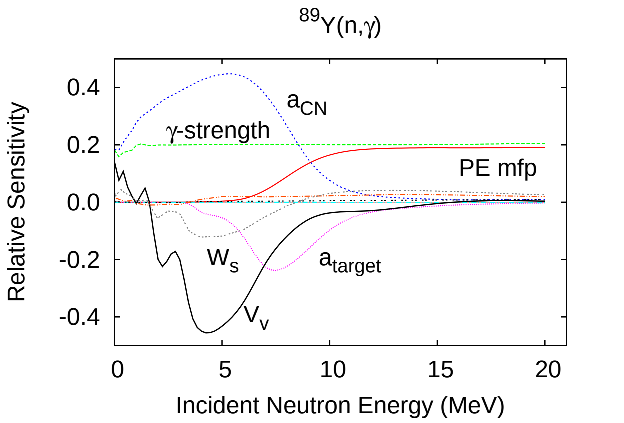

Fig. 5. Relative sensitivity of neutron capture on ^{89}Y to the 10% perturbation of various model parameters (γ-strenght perturbed by 20%).

If such an adjustment is done on a large scale it should produce improved global set of model parameters.

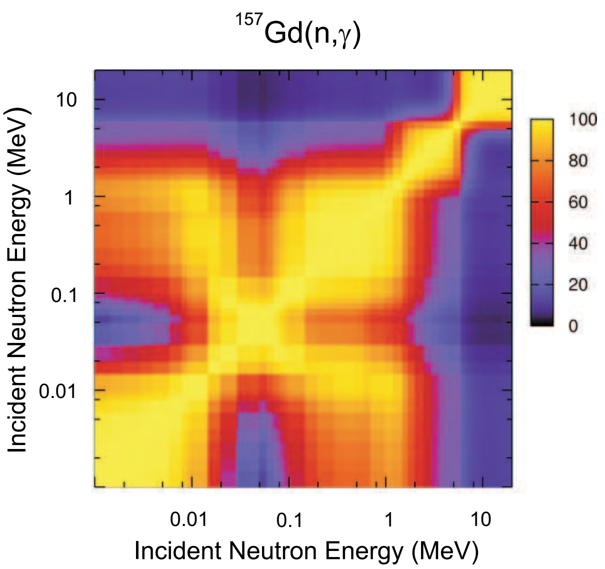

Fig. 6. Correlation matrix for the ^{157}Gd neutron capture cross sections in the fast neutron region obtained with the EMPIRE-KALMAN method.

6 Ultimate vision

Modern evaluations tend to rely on nuclear reaction theory with experimental data being critical for the calibration of model parameters. Then the library is validated against integral measurements, generally much more precise than the microscopic ones. However, integral measurements integrate over many nuclides, reactions and incident energies that makes tracing eventual discrepancies back to the microscopic data generally very difficult and in most cases inconclusive.

An alternative approach is to achieve such precision in the microscopic data that there is no need for any adjustments to reproduce integral experiments. This can be attempted by incorporating integral measurements into the evaluation procedure. Recent progress in nuclear reaction modeling, qualitative jump in the computing resources, current status of modern transport calculation codes, and availability of key libraries such as RIPL (model parameters), EXFOR (microscopic experimental data) as well as the comprehensive compilation of benchmark experiments (ICSBEP) provide justified expectation that such an ambition task is technically feasible. Our confidence builds on the follwing:

– simultaneous evaluation (model calculations) of the entire library (or a considerable part of it) and its benchmarking against hundreds of integral measurements will considerably increase constrains on the adjustments of the microscopic data,
– adjustment of model parameters instead of cross sections will greatly reduce number of quantities to be adjusted reinforcing the effect of the previous point,
– comprehensive sensitivity calculations coupled to the advanced statistical methods (e.g., KALMAN filtering) will ensure that the adjustment is optimal.

Such a project, known as Global Nuclear Data Initiative, has recently been gaining support within the US nuclear data community.

7 Conclusions

The EMPIRE code has reached sufficient level of robustness and reliability to provide substantial support for the development of ENDF/B-VII.0. Several important extensions and improvements were introduced. Recently, the code has been embracing new territories: neutron resonances and the covariances. Our vision for future goes even further - consider the library as a single entity, rather than as the collection of isotopes. The dream is to construct *consistent* set of (short) input files that, together with the nuclear reaction code, could replace the entire library of cross sections. Ultimately, if the physics is right, there should be only one input!

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