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Extension of the EMPIRE Code to the Resonance Region

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Abstract. The preliminary version of a new module has been developed to be added to a nuclear reaction model code EMPIRE to allow for an evaluation of neutron cross sections in a resonance region. It automates most of the evaluation procedures and can be executed within EMPIRE or as a stand-alone program. The module includes a graphic user interface (GUI) and a number of codes and scripts that read individual, as well as average, resonance parameters from the Atlas of Neutron Resonances and other physical constants from RIPL-2, perform an analysis of the available resonances, carry out statistical distributions, and compute cross sections in resolved and unresolved resonance regions which are then compared with experimental data. The module also provides an ENDF-formatted file for a resonance region and various plots allowing for a verification of the procedure. The formatted file can be integrated later into the final ENDF-6 file as generated by the EMPIRE code. However, as a preliminary version, extensive testing and further improvements are needed before this new capability can be incorporated into the production version of EMPIRE.

1 Introduction

Currently, the evaluation of cross sections in a resonance region is accomplished by using the several different codes by following a complex procedure. The resolved resonance parameters for each nuclide are provided separately as a computerized data file called BNL325.TXT and each code requires one or more input files. Hence, there is a strong possibility of causing a human error while conducting the several stages involved in evaluation tasks.

The preliminary version of a new module has been developed to be added to a nuclear reaction model code EMPIRE [1] to allow for an easier evaluation of neutron cross sections in a resonance region. Our fundamental design goal is to automate most of the procedures involved in evaluation tasks. It is designed such that it can be executed within EMPIRE or as a stand-alone program. The module performs an analysis of the available resonances, provides statistical distributions, and computes cross sections in resolved and unresolved resonance regions. The module also provides an ENDF-6 formatted file [2] for a resonance region and various plots allowing for a verification of the procedure. The formatted file can be integrated later into the final ENDF-6 file as generated by the EMPIRE code. In the present paper, use of the resonance module and some sample cases are presented.

2 Architecture of the resonance module

The resonance module consists of a graphic user interface (GUI) and a number of codes such as SCANR, PTANAL [3], WRIURR [3], RECENT [4] and SIGMA1 [5] and scripts that read resonance parameters and other physical constants, perform an analysis of the available resonances, provide statistical distributions and compute cross sections in resolved and unresolved resonance regions which are then compared with the available evaluated cross sections and experimental data.

Fig. 1. The screen shot of GUI main control panel.

At a start-up, the module reads all the necessary data for the target nucleus including individual, as well as average, resonance parameters from the Atlas of Neutron Resonances [6] and other physical constants from RIPL-2 [7] and displays them on the screen. The evaluator has the possibility to

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modify the nuclear parameters before performing calculations in the resolved and unresolved regions. Figure 1 shows an example screen for Ni-60. The left part of the screen is the editable input area. The evaluator has a chance to start the new evaluation for another nuclide by entering the new ZA and MAT and then pressing the 'Reload' button. The right part of the screen provides the buttons for performing various plots for an analysis and comparison with the experimental data and the available evaluated cross sections. The lower bottom screen shows the various codes which can be scheduled to run.

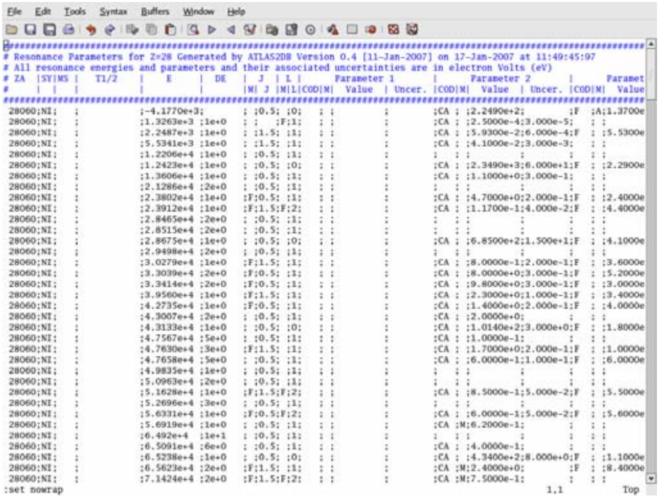

Fig 2. The screen capture of resolved resonance parameter.

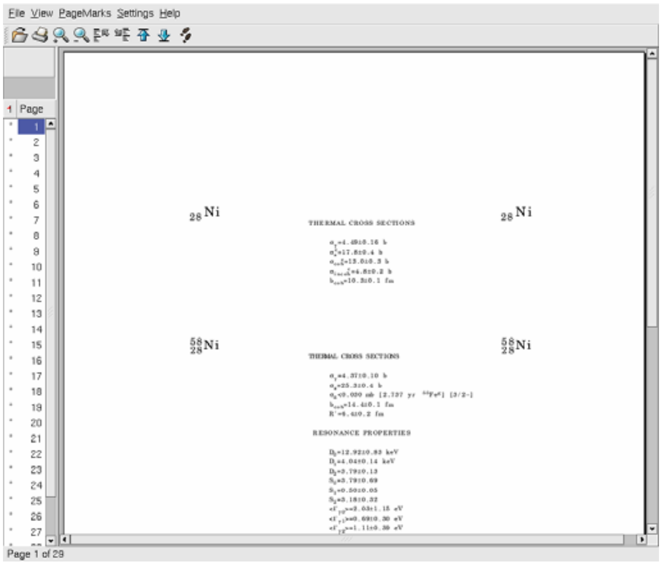

Fig. 3. The image of Atlas of Neutron Resonances.

The evaluator also has a chance of editing the resolved resonance parameters if needed. Figure 2 shows the screen displayed after choosing the button labelled 'Resonance parameters'. The modified parameter table is stored on the local directory and can be reverted to the original one anytime. The program for viewing the parameter table (and also other visual graphics) can be customized as in the EMPIRE code. For a verification purpose, the scanned images of Atlas of Neutron Resonances can also be displayed by pressing the button labelled 'Atlas of Neutron Resonances' as shown in Fig. 3.

3 Calculation method and procedure

The PTANAL and WRIURR codes which have been slightly modified for the resonance module are used for the calculations of the resonance parameters in the resolved and unresolved energy regions, respectively.

The PTANAL code assigns the angular momentum and spin values, which have not been determined from the measurements, to resonances by using the Bayesian method and a random assignment method, respectively. It also assigns the radiative width which is obtained by averaging the measured radiative widths to the resonances with no measured one. In addition, the reduced resonance widths are analysed and fitted to the Porter-Thomas distribution [8] which helps in the determination of the average resonance parameters such as a level spacing and neutron strength function for s- and p-waves. The current version reads the resonance parameters from the Atlas of Neutron Resonances and constructs the ENDF-6 formatted file. The WRIURR code appends the average resonance parameters for the unresolved resonance region to the ENDF file. The new version accepts the power of an energy dependent function for the gamma width as an input. The gamma width at the resonance energy E is then calculated by the following equation.

$$\Gamma_g(E) = \Gamma_g \left[\frac{B_n - \Delta + E}{B_n - \Delta} \right]^{Gp} . \qquad (1)$$

where Γ_g is the average gamma width, Δ is the pairing energy, B_n is the binding energy and G_p is the arbitrary exponent. The default exponent is currently 2.5. The pairing energy can be calculated in the code.

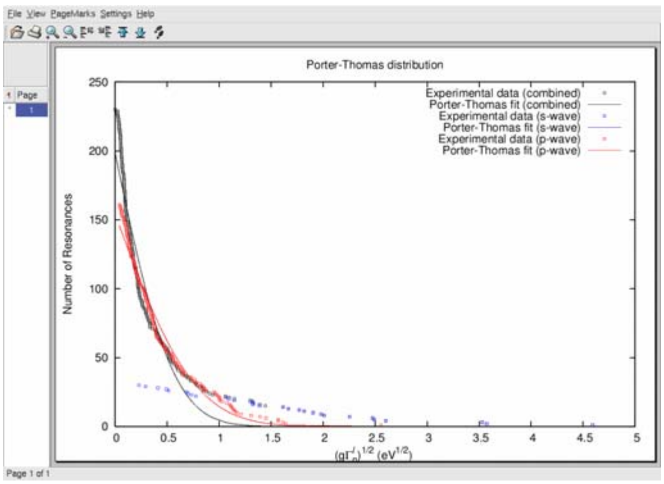

Fig. 4. Graphical display of the Porter-Thomas distribution.

Figure 4 shows a graphical display of the Porter-Thomas distribution provided by the resonance module as a result of reading the output of the PTANAL code.

The SCANR code has been newly developed and is used for a graphical analysis of the resonance energies, which helps in the determination of the upper boundary of the resolved resonance region (see fig. 5). The trial value of the upper boundary can be given as an optional input. When it is given, a search for the upper boundary is performed from that point.

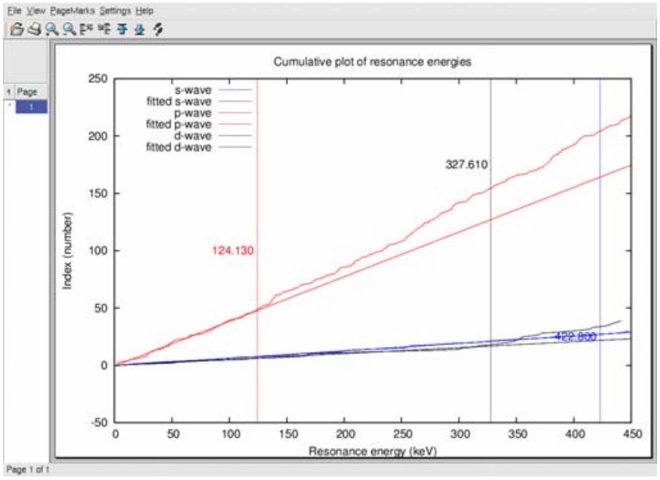

Fig. 5. The cumulative plot of resonance energies.

The calculated resonance parameters with the PTANAL and WRIURR codes can then be constructed as point-wise cross sections by invoking auxiliary codes such as RECENT and SIGMA1, and compared with the experimental data. At this stage, the evaluator also can choose any or all of the available evaluated cross sections including ENDF/B-VII [9], JENDL-3.3 [10] and JEFF-3.1 [11] (see figs. 6 and 7) to be compared with the calculated data.

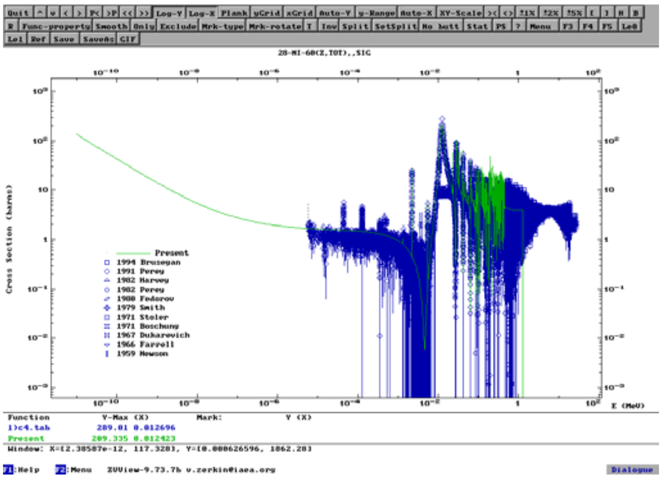

Fig. 6. The screen shot of calculated elastic cross sections compared with the experimental data. The results also can be compared with the evaluated cross sections if any.

All the tasks except for the modification of the default values for the standard resonance parameters and physical constants are executed with simple mouse clicks. The module also provides an ENDF-6 formatted file for the resonance region. The formatted file can be integrated later into the final ENDF-6 file as generated by the EMPIRE code if the module is executed within the EMPIRE code.

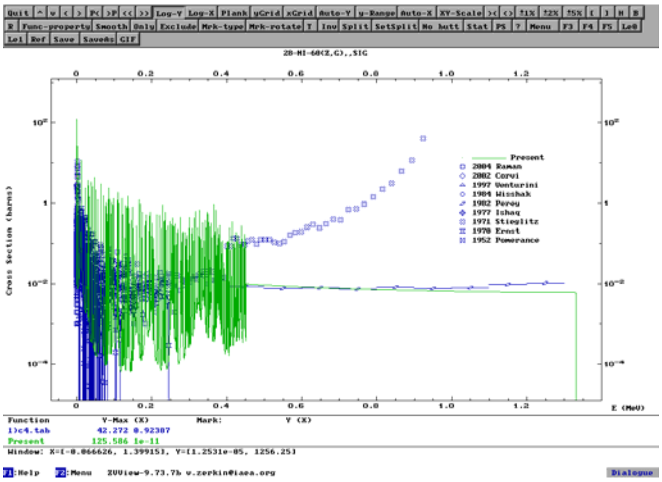

Fig. 7. The screen shot of calculated capture cross sections compared with the experimental data.

4 Summary and Future Works

The preliminary version of a new module has been developed for an evaluation of the cross sections in resolved and unresolved resonance regions. It can automate most of the evaluation procedures and can be executed within EMPIRE or as a stand-alone program. When it is used as connected to the EMPIRE code, a single ENDF-6 formatted file can be obtained for a full energy region. As most of the tasks are performed with a few simple mouse clicks on the GUI control panel providing various plots that help the evaluator check on the validity of the calculation results, it will minimize the possible human error factor and improve the productivity and efficiency of the evaluation tasks.

In the current version, the SCANR code searches and suggests the upper boundary of a resolved resonance region by comparing the chi squares between the experimentally determined resolved resonance energies and the fitted ones. While the sample evaluation works for some nuclides showed that the algorithm implemented in the SCANR code predicted reasonable values, some other cases indicated the necessity for an improvement. An improvement to the algorithm will be made by inspecting the results of future evaluation works for various other nuclides. Moreover, extensive testing and further improvements are needed before this new capability can be incorporated into the production version of EMPIRE

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