Recent Development and Validation of the Nuclear Reaction Code EMPIRE

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Recent extensions of the EMPIRE-II code system are presented. These include link to the Coupled Channels code ECIS, second chance preequilibrium emission, Monte Carlo preequilibrium (HMS), width fluctuations (HRTW), improvements in the γ-ray strength functions, link to the omp segment of RIPL, calculation of recoil spectra, and possibilities to plot angular distributions, energy spectra and double differential cross sections using PLOTC4 and/or ZVView package. The emphasis is on the validation of the code through comparison with experimental data and recent application to nuclear data evaluation.

KEYWORDS: neutron cross-sections, nuclear data evaluation, model calculations, statistical model, widths fluctuation, coupled channel model, exciton model, preequilibrium, recoils

I. Introduction

EMPIRE-II belongs to the new generation of statistical model codes. It was officially released in March 1999 (version 2.13 Trieste). Since then, the code has been under constant and intensive development, which lead to significant improvements and extensions. The code is intended as a general theoretical tool to be used in basic research and nuclear data evaluation for calculation of nuclear reactions in the broad range of incident energies and projectiles. It was designed to contain state of art nuclear reaction modeling, being at the same time very easy to use. A full ENDF-6 formatted file and its graphical comparison with the available experimental data can be obtained with just a few mouse clicks and key strokes.

The most recent version EMPIRE-2.16 (Montenotte) includes major nuclear reaction mechanisms, such as optical model (SCAT2), coupled channels (ECIS), Multistep Direct (ORION + TRISTAN), NVWY Multistep Compound, Monte Carlo preequilibrium emission, and the full featured Hauser-Feshbach model with widths fluctuation correction (HRTW). Heavy Ion fusion cross section can be calculated within the simplified coupled channels approach (CCFUS). A comprehensive library of input parameters covers nuclear masses, optical model parameters, ground state deformations, discrete levels and decay schemes, level densities, fission barriers (BARFIT), moments of inertia (MOMFIT), and γ-ray strength functions. Effects of the dynamic deformation of a fast rotating nucleus can be taken into account in the calculations. The results can be converted into the ENDF-6 format using the accompanying code EMPEND by A. Trkov. The package includes the full EXFOR library of experimental data. Relevant EXFOR entries are automatically retrieved during the calculations. By default, plots comparing experimental results with the calculated ones are produced using the extended PLOTC4 code linked to the rest of the system through a series of preprocessing codes and bash-shell scripts. Interactive plotting is possible through the powerful ZVView package. Easy operation of the whole system is assured by the graphic user interface written in Tcl/Tk.

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II. Recent EMPIRE-II extensions

1. Link to RIPL

Interface to RIPL[1)] optical model segment was added to Empire by R. Capote. RIPL OM parameters are selected via a single input line with an OMPOT keyword. For a given RIPL potential the corresponding OMPAR.RIPL file is created. This file can be edited in order to change OM parameters from the RIPL recommended values if desired. We note that RIPL coupled channel potentials also include the relevant collective discrete levels along with appropriate deformation parameters.

2. Coupled Channel code ECIS

ECIS[2)] is a well known and highly respected code for calculations within the generalized (deformed) optical model and coupled channels model (CCM). ECIS is important for modeling reactions on deformed nuclei, in particular, for description of strong population of collective discrete levels in the (n,n') channel. ECIS-95 was added to EMPIRE as its new extensive module by R. Capote in February 2001. This implementation features automatic preparation of the ECIS input. It uses RIPL[1)] library and resorts to the EMPIRE built-in discrete level schemes and deformation parameters if necessary.

ECIS can be invoked by EMPIRE in three different ways, using input directive DIRECT=1,2 and 3.

- DIRECT 1. Population of (n,n') or (p,p') discrete collective levels is calculated within CCM. This gives exact direct cross section. However, spherical transmission coefficients provided by SCAT2 are used in the whole energy grid for subsequent preequilibrium and HF calculations.
- DIRECT 2. Population of (n,n') or (p,p') collective levels is calculated within CCM as above. Importantly, CCM is used consistently, considering ground state and coupled levels, to calculate all necessary transmission coefficients for subsequent preequilibrium and HF calculations. This option is more accurate but calculation time

is considerably longer.

- DIRECT 3. Population of (n,n') or (p,p') collective levels is calculated using DWBA method. This gives approximate direct cross section but is a useful option when coupled channel optical model potential is not available. The spherical transmission coefficients provided by SCAT2 are used for the whole energy grid in preequilibrium and HF calculations.

3. Exciton model module DEGAS

This module was incorporated to improve (n,γ) reactions for fast neutrons and add the capability of predicting spectra for charge exchange reaction that are not provided by the current implementation of the MSD model (ORION&TRISTAN). DEGAS is the exciton model code with angular-momentum conservation. It was written by E. Běták (Bratislava, Slovakia) as an improved version of the code PEGAS[3] by E. Běták and P. Obložinský. DEGAS was added to EMPIRE by P. Obložinský (BNL) in February 2001.

By comparing practically all available experimental data for (n,γ) and (p,γ) excitation functions in the incident energy range 8-20 MeV the Bratislava-Ljubljana collaboration demonstrated[4] that DEGAS results are very close to the more microscopic direct-semidirect capture model.

4. Monte Carlo preequilibrium emission (HMS)

Inclusion of the Monte Carlo preequilibrium module (DDHMS coded by M.B. Chadwick) extends useful energy range of EMPIRE up to the intended limit of about 200 MeV for nucleon induced reactions. The HMS model, developed by M. Blann,[5] is an exciton model inspired treatment of the intranuclear cascade. Each exciton is allowed to create a new particle-hole pair or escape the composite nucleus if the exciton is of a particle (rather than hole) type. The Monte Carlo method is used to decide whether the interaction counterpart is a neutron or proton, to select particle-hole pair energy and to choose exciton directions. The cascade is terminated when all excitons fall below binding energy. The HMS model needs only 1p-1h level densities, therefore it avoids inconsistent use of multi-exciton level densities typical of classical preequilibrium models. An important feature of the model is that it takes into account unlimited number of multi-chance preequilibrium emissions and observes angular momentum and linear momentum coupling. It provides double differential emission spectra of neutrons and protons, spin and excitation energy dependent populations of residuals, and excitation energy dependent recoil spectra. These results are transferred onto EMPIRE arrays and used as a starting point for the subsequent compound nucleus decay.

5. Second-chance preequilibrium emission after MSD

A simple treatment of the second-chance preequilibrium emission has been incorporated in connection with the MSD (TUL) model. A semi-classical formulation proposed by M. Chadwick[6] has been adopted. The current implementation assumes that MSD emission leave residual nucleus containing a single particle-hole pair of energy equal to the excitation energy of the residual. The excited particle (neutron or proton) is given a chance to escape the nucleus. The emission rate is defined by the product of the related s-wave transmission coefficient and the probability for the exciton to have excitation energy compatible with the channel energy. Angular momentum coupling assumes 1p-1h spin distribution for the exciton pair. This treatment allows to account only for the second-chance emission. Thus it extends applicability of the MSD model up to the energies at which higher order emissions can still be neglected. In general it results in a modest increase of the central part of the emission spectra.

6. Width fluctuations (HRTW)

The widths fluctuation correction to the Hauser-Feshbach model was added by M. Herman to improve code performance at low incident energies. The HRTW[7] model with improved elastic enhancement factor[8] has been used. The latter was designed to treat cases when strong channels are mixed with the large number of very weak ones. The HRTW replaces optical model transmission coefficients with the effective ones that take into account unitarity of the S-matrix when the elastic channel strength is increased by the elastic enhancement factor. All channels are divided into strong ($T_l \geq 0.0001$) and week ones ($T_l < 0.0001$). For the strong channels effective transmission coefficients are calculated by iteration. For the week ones only the first iteration is applied. Particle channels are treated explicitly while γ-channels are lumped into one or more fictitious channels.The HRTW model is applied by default below 5 MeV incident energy.

7. Model compatibility and priorities

EMPIRE allows to include different preequilibrium models in a single calculation run, which rises the problem of double-counting. In general, ECIS is compatible with DEGAS and HMS as the latter two do not calculate collective excitations. By the same token ECIS in not compatible with MSD as both include collectivity of discrete levels. However, ECIS and MSD can be combined providing that only the continuum contribution from MSD is retained.

When combining different models the priorities are the following:

- ECIS provides inelastic scattering to collective levels independently of settings for the remaining models.
- MSD provides inelastic continuum independently of other settings. Inelastic to discrete levels is suppressed if ECIS is active.
- MSC results are taken for inelastic and charge-exchange to continuum if not suppressed by use of DEGAS or HMS.
- DEGAS provides inelastic and charge-exchange to continuum and to discrete levels if MSD and MSC are not active. Otherwise only charge-exchange contribution is used. Gamma emission is used if not provided by MSC.
- HMS provides inelastic and charge-exchange to continuum and to discrete levels if MSD and MSC are not

active. Otherwise only charge-exchange contribution is used. Suppresses DEGAS results for particle emission if DEGAS is active. Does not provide γ-rays, thus DEGAS or MSC results are taken.

At incident energies below 20-30 MeV the best results are expected by combining the first 4 models. At higher incident energies these should be replaced by the HMS model, which accounts for the multiple preequilibrium emission.

8. Recoil spectra

Capability of calculating recoil spectra has been extended to all residuals independently of the number of emitted particles. In addition, correlation between the recoil energy and the excitation energy of a residual is preserved. For each light particle emission an appropriate contribution to the recoil spectrum is stored in the excitation energy dependent array. This is done by vector addition of velocities. The velocity distributions are generally forward peaked for the first emission and isotropic for the other ones. The actual angular distributions of recoils are not provided but their influence on energy spectra is taken into account. The recoil spectra are given in the laboratory system and include center of mass motion. This approach is superior to deducing recoil spectra from the light particle emission spectra, which neglects correlations along the deexcitation cascade.

9. Plotting capabilities

All pertinent experimental data in EXFOR are retrieved by the code during the first run and plotted against the ENDF formatted file using the ENDF Pre-Processing codes (Pre-Pro) and the pair of codes X4toC4 and PLOTC4 by D.E. Cullen. The codes are called from EMPIRE in a transparent way by internal scripts.

The X4TOC4 and PLOTC4 codes, as used in EMPIRE-2.16, have been extended and incorporated into the ENDF Data Verification Package (ENDVER) by A. Trkov and D.E.Cullen to enable plotting of angular distributions and double-differential cross sections. If experimental data exist appropriate plots are automatically generated at the end of each run. In addition, plotting capabilities have been greatly enhanced by incorporating the graphic package ZVView [9] by V. Zerkin. This software is operated from the EMPIRE Graphic User Interface and is able to produce publication quality plots with extended possibilities for manual interaction. The options include change of scale, excluding selected data set from the plot, displaying data point values, basic statistical analysis, changing plot symbols and colors, data fitting, smoothing and others. ZVView plots can also be combined to include different reactions on the same plot. In the current implementation only cross sections (MF=3) can be plotted with ZVView. Work is in progress to include angular distributions and double-differential cross sections.

III. Testing the predictive power

Predictive power of each new version of EMPIRE-II is routinely tested by calculating a set of reactions using default model parameters. This set contains 24 targets: ^{31}P, ^{40}Ca, ^{47}Ti, ^{52}Cr, ^{55}Mn, ^{58}Ni, ^{63}Cu, ^{71}Ga, ^{80}Se, ^{92}Mo, ^{93}Nb, ^{100}Mo, ^{109}Ag, ^{114}Cd, ^{124}Sn, ^{127}I, ^{133}Cs, ^{140}Ce, ^{153}Eu, ^{169}Tm, ^{186}W, ^{197}Au, ^{208}Pb, and ^{238}U. The 33 incident neutron energies cover the range from 1 keV up to 20 MeV. The calculated reactions are (n, xn yp zα), with x=0,1,2, y=0,1, and z=0,1. Multistep Direct and Multistep Compound models are used in the neutron channel while exciton model (DEGAS) accounts for the preequilibrium emission of protons. Standard number of 10 discrete levels in each nucleus is considered and the EMPIRE specific level densities are used in the continuum. Spherical optical model potential by Wilmore-Hodgson [11] is used for neutrons. We stress again that all input parameters are default and no adjustment of their values is attempted. The results are converted into the ENDF formatted file and automatically plotted against experimental data. This includes cross sections, angular distributions and double-

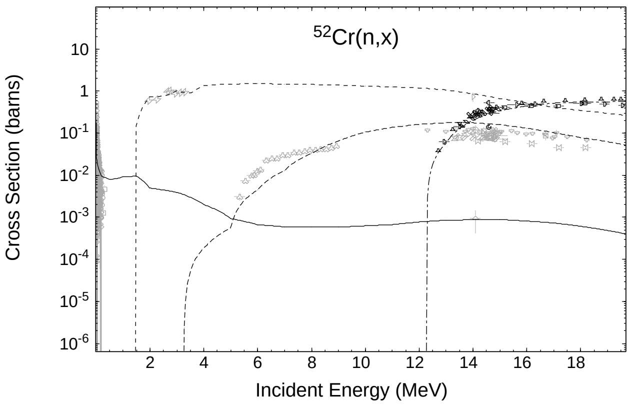

Fig. 1 Default calculations for radiative capture (solid line), inelastic scattering (dotted line), (n,2n) (dashed line), and (n,p) (dashed-dotted line) reactions on ^{52}Cr compared with experimental data from EXFOR.

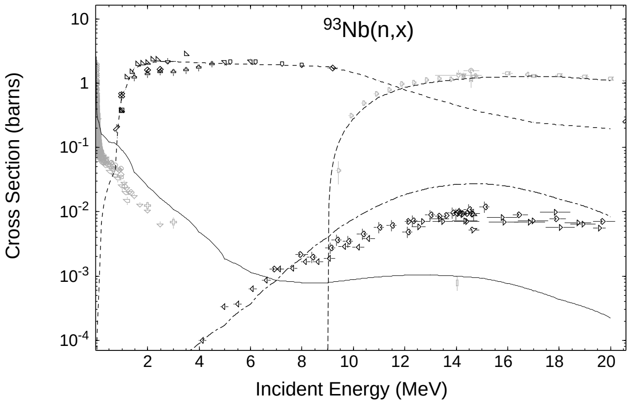

Fig. 2 Default calculations for radiative capture (solid line), inelastic scattering (dotted line), (n,2n) (dashed line), and (n,p) (dashed-dotted line) reactions on ^{93}Nb compared with experimental data from EXFOR.

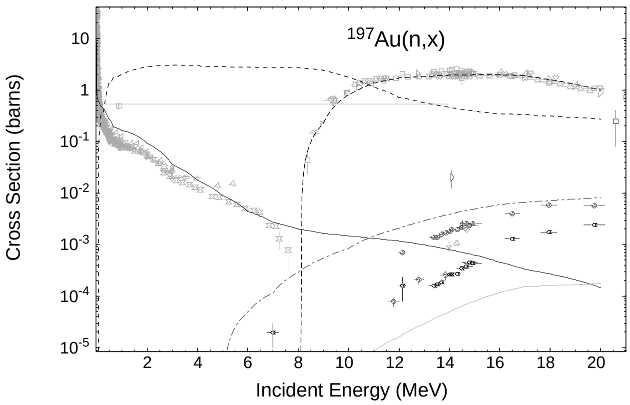

Fig. 3 Default calculations for radiative capture (solid line), inelastic scattering (dotted line), (n,2n) (dashed line), (n,p) (dashed-dotted line) and (n,α) (solid gray line, the lowest) reactions on ^{197}Au compared with experimental data from EXFOR.

differential cross sections whenever available.

Typical results are shown in Figs. 1, 2, and 3. Taking into account 'blind' nature of these calculations the code performs very well for neutron capture, inelastic scattering and (n,2n) reactions. It should be noted that emission spectrum of the first neutron is substantially harder than the one obtained with classical nuclear models. It is due to the enhanced strength of transitions to the collective (vibrational) states in the MSD-TUL model. This feature actually allows for very reasonable reproduction of double-differential and angle-integrated spectra for neutrons. Agreement for the (n,p) cross sections is reasonable but generally worse than for the above mentioned reactions. Comparison of the (n,α) cross sections is rather unfavorable, with exception of the nuclei around A=60 for which the code performs exceptionally well. In particular, the (n,α) cross sections are dramatically underestimated for the heavy nuclei. This is mostly due to the preequilibrium emission of α-particles, which is not included in the present version of the code. In addition, optical model parameters for α-particles are very uncertain. This might be the main reason of discrepancies for $A < 100$ nuclei. Scarcity of the data for (n,np) and (n,nα) reactions does not allow to draw decisive conclusions on these rather weak channels.

IV. Application to nuclear data evaluation

Recent versions of EMPIRE have been used in the BNL-KAERI evaluations[10] of 19 fission product isotopes. This exercise provided a thorough test of the code and helped to correct some bugs which could only be detected in practical, large scale calculations. The code proved to be flexible enough for use in nuclear data evaluation. In this respect, the possibility of combining different nuclear models turned out essential. The evaluation work was substantially speeded up by simplicity of the input and automatic ENDF formatting followed by graphical comparison with experimental data. Some of these results are presented in a dedicated contribution[10] to this Conference.

V. Conclusions

EMPIRE-2.16 (Montenotte) is a powerful tool for predicting nuclear reaction cross sections. It can be applied for various projectiles (including Heavy Ions) in the broad range of incident energies. In spite of the advanced modeling, and numerous mechanisms included, the code is exceptionally user friendly. In Section 3 we have demonstrated that the results of calculations using all default parameters are quite reasonable for the most important reaction channels up to 20 MeV. This comparison shows a considerable predictive power of the code. These results can be further improved (still without any adjustment) by selecting individual parameters better suited for the particular cases (such as number of discrete levels, optical model potentials, etc.).

Future development of the code will address weak points of the current version. First of all, treatment of the fission channel (presently only suited for Heavy Ion induced reactions) will be improved. Next, preequilibrium emission of clusters will be considered. Closer integration with the RIPL library is also foreseen.

We would like to stress that EMPIRE is the result of truly international and voluntary(!) collaboration, which builds upon free software made available by various developers. Present status of the code demonstrates enormous potential of such an approach in nuclear data applications.

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