Recent Developments of the Nuclear Reaction Model Code Empire

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Abstract. Recent extensions and improvements of the EMPIRE code system are outlined. They add to the code new capabilities such as fission of actinides, preequilibrium emission of clusters, photo-nuclear reactions, and reactions on excited targets. These features, along with improved ENDF formating, exclusive spectra and recoils make the forthcoming 2.19 release a complete tool for evaluation of nuclear data at incident energies above the resonance region.

INTRODUCTION

EMPIRE belongs to a new generation of nuclear reaction codes, and is intended as a general theoretical tool to be used in basic research and nuclear data evaluation over a broad range of incident energies and projectiles. It was designed to contain up to date nuclear reaction models as well as being easy to use. The currently available version EMPIRE-2.18 (Mondovi)[1] includes major nuclear reaction mechanisms, such as optical model (SCAT2[2]), coupled channels (ECIS[3]), Multistep Direct[4] (ORION + TRISTAN), NVWY Multistep Compound[5], Monte Carlo pre-equilibrium emission[6, 7], and the full featured Hauser-Feshbach model with widths fluctuation correction (HRTW[8]). 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[9]), moments of inertia (MOMFIT[9]), and γ-ray strength functions. The results can be converted into the ENDF-6 format using the accompanying code EMPEND . The package includes full EXFOR library of experimental data that are automatically retrieved during the calculations. By default, plots comparing experimental results with the calculated data are produced using the extended PLOTC4[10] code linked to the rest of the system through a series of pre-processing codes[11] and bash-shell scripts. Interactive plotting is possible through the powerful ZVView package[12]. Simple operation of the whole system is ensured by the graphic user interface (GUI).

NEW FEATURES

EMPIRE-2.19 (Lodi), the version to be released in the near future, will include:

- multi-modal fission through multi-humped barriers,
- exciton model for cluster emission (Iwamoto-Harada),
- suite of γ-ray strength functions from RIPL-2,
- photo-nuclear reactions,
- reactions on excited targets,
- new algorithm for calculation of exclusive spectra and recoils,
- simultaneous calculations of Coupled-Channel and DWBA contributions,
- merging resonance parameters into the final ENDF file,
- improved ENDF formatting and its verification,
- matured version of the new GUI,
- GUI assisted fitting of optical model parameters,
- chain of checking codes CHECKR, FIZCON, and PSYCHE,
- automatic and manual access to the CSISRS/EXFOR database operated under MySQL,

along with a number of minor improvements and bug fixes. Some of these extensions are outlined below.

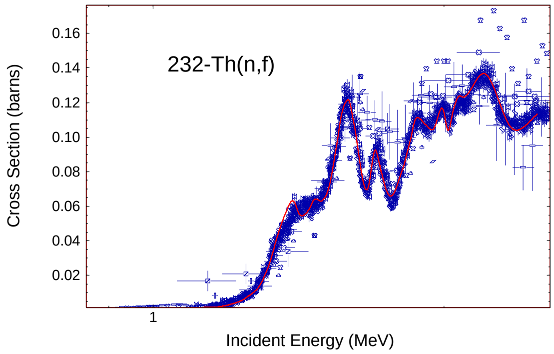

FIGURE 1. EMPIRE-2.19 results for neutron induced fission of ^{2}32Th compared with experimental data showing code capability of reproducing complicated structure in the cross section

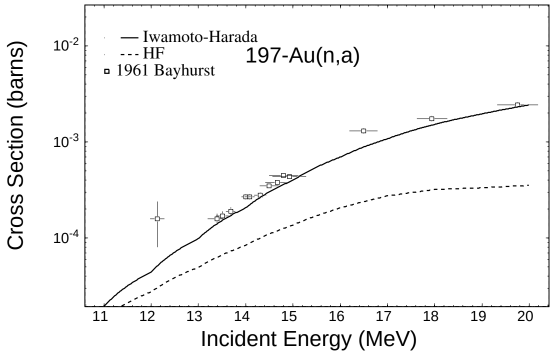

FIGURE 2. Improvement achieved with the Iwamoto-Harada model for ^{179}Au(n,α) reaction.

Fission

Modeling of the fission channel in the EMPIRE-2.18 code was only adequate for heavy ion induced reactions. Version 2.19 (Lodi) introduces an advanced fission formalism applicable also to the multi-chance fission induced by low energy nucleons.

Light particle induced fission proceeds through the formation of the compound nucleus treated in EMPIRE-II within Hauser-Feshbach and HRTW models. The expression for the fission probability, as used in the 2.19 version, is derived in the frame of the optical model for fission. It describes the transmission through a multi-humped barrier starting from the sub-barrier excitation energies. Using this generalized relation, it is possible to reproduce experimental fission cross sections (including the resonant structure observed in fertile nuclei) and to set up a general procedure for determining parameters describing fission barriers associated with the transition states.

In the first run EMPIRE automatically creates auxiliary input file with parameters describing discrete fission barriers and level densities at the saddle points. These values are taken from RIPL-2, from internal systematics, or are calculated by the code. For the level densities at the saddle points the HF-BCS results of RIPL-2 or the dynamical approach specific to EMPIRE (accounting for collective enhancements and nuclear shape asymmetry at each saddle) can be used. The user can easily modify fission related parameters by editing the existing input file.

Encouraging results (see Fig. 1) show that improvement of the fission channel extends applicability of the EMPIRE code to the interaction of low energy neutrons with the actinides, which is of primary importance for various applications.

Preequilibrium emission of clusters

EMPIRE-2.19 acquired the capability of using preequilibrium mechanism for clusters in the incoming and outgoing channels by including the Iwamoto-Harada model [13] parameterised and improved in Refs. [14, 15, 16]. In this model, the formation probability of a cluster takes into account excitons below and above the Fermi surface and avoids free parameters. In Fig. 2 we demonstrate the essential improvement which Iwamoto-Harada model brings into the treatment of α-particle emission in the ^{179}Au(n,α) reaction.

γ-ray strength functions

Versatility of the EMPIRE has been extended by incorporating 6 approaches to the E1 γ-ray strength functions recently provided by the RIPL-2 project. These include: (i) standard Lorentzian (SLO), (ii)Enhanced Generalized Lorentzian (EGLO) [17], (iii) Generalized Fermi Liquid model (GFL) [18], and (iv) three versions (MLO1, MLO2, and MLO3) of the Modified Lorentzian model by Plujko [19] that are all based on the thermodynamic pole approximation and differ in the treatment of the response functions and collisional relaxation. Preliminary tests seem to favor GFL and MLO1 approaches.

Photo-reactions

The new suit of E1 γ-ray strength functions can be used in the incoming channel to determine photoabsorption cross section and its spin distribution. The input parameters (width, strength and position of the GDR) are taken from the RIPL-2 library. Contributions from the E2 and M1 transitions are also allowed. Subsequent decay of the compound nucleus is treated within the stan-

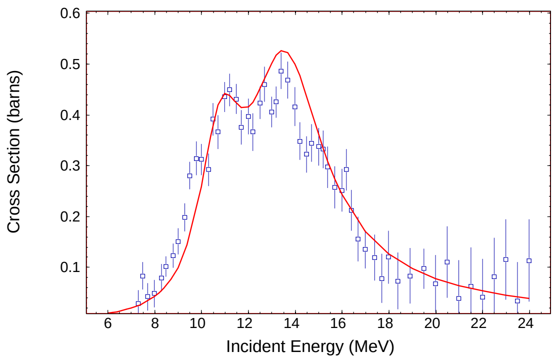

FIGURE 3. Comparison of EMPIRE-2.19 calculations and experimental data for photo-absorption on $^{2}35U$

dard Hauser-Feshbach model. Figure 3 compares calculated and experimental photo-absorption cross sections on $^{2}35U$ using MLO1 γ-ray strength function.

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Reactions on excited targets

EMPIRE-2.19 accepts targets that are excited to any of the available discrete levels. In such case, spin of this state rather than the one of the ground state is used for the calculation of the compound nucleus spin distribution and the excitation energy is increased by the the excitation energy of the target. Subsequent decay follows standard Hauser-Feshbach approach.

Exclusive spectra

Standard ENDF-6 format requires exclusive particle spectra being coded in the formatted files. For example, the neutron spectrum associated with the (n,2n) reaction must include both the first and the second neutron that were emitted to create appropriate (n,2n) residue. Consequently, the first emitted neutron, if followed by any other particle emission, must not be counted in the (n,n') spectrum. This requirement is a challenge for the standard model codes that usually do not carry over enough history to disentangle emission spectra into the exclusive ones.

The approximation employed in EMPIRE-2.18 assumed that no gammas are emitted prior to any particle emission. For heavier nuclei this assumption breaks down already at incident energies below 20 MeV leading to negative particle and γ spectra. In addition, this approach was limited to two subsequent emissions (e.g., (n,3n) reactions could not be treated).

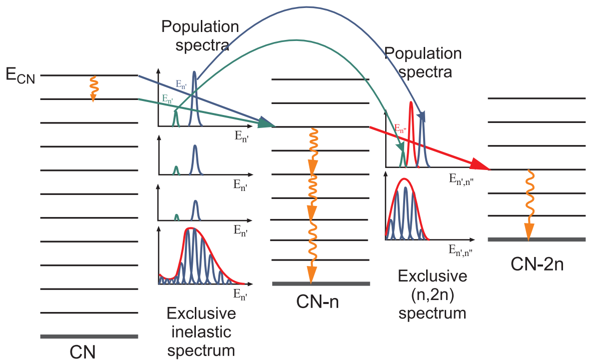

FIGURE 4. Schematic representation of the algorithm for calculation of exclusive spectra (see text for details)

For the 2.19 version of the code a completely new approach, based on the concept of the 'population spectra', has been developed. Figure 4 sketches the procedure involved in the calculations. The separate 'population spectra' are associated with each energy bin in the discretized continuum. They represent cumulative spectra for each type of ejectile that contributed to the population of a given energy bin in the residue.

Since all particles in the cascading emissions should be counted in the spectrum of the final residue, each time a particle is emitted it removes a part of the population spectra in the bin from which it originates and deposits it on the population spectrum of the final bin. This part has the original spectral shape and its integral is proportional to the intensity of the considered transition. The particle itself contributes to the final bin population spectrum a spike at the energy with which particle was emitted. Once all transitions from a given bin are processed, the population spectrum of the bin is totally depleted and distributed over population spectra of the final bins.

In this calculational scheme, γ-transitions play a particular role of transferring population spectra down to the excitations stable against particle emission. These contributions (undepleted) sum up on the residual nucleus ground state to form exclusive spectra associated with the residue.

The algorithm can be applied for any number of subsequent emissions and ejectiles, and can accommodate any reaction mechanism. The only approximations involved in such calculations are neglect of spin and lack of correlations between subsequent emissions. The latter assumption is consistent with the statistical theory of nuclear reactions, while the former one could easily be removed but at the cost of very involved calculations.

The new algorithm spin off is a possibility to resolve different reactions leading to the same residual nucleus (e.g., cross sections for the (n,d) and (n,np) reactions can be determined)

Recoils

Spectra of recoils are calculated using an algorithm analogous to the one described above for the exclusive spectra. Differently from the 2.18 version, this approach in now used independently of the formatting option. The recoil spectra are calculated in the CM system and account for the boost due to the center of mass motion.

Coupled-Channel and DWBA

In certain cases, reproduction of the inelastic scattering to discrete levels calls for a direct reaction contributions to many levels, including those that do not belong to the ground state rotational or vibrational band. The 2.19 version allows to treat certain group of levels within the Coupled-Channel approach and the remaining ones within the DWBA in a single run. The results of both models are then automatically combined and no manual post processing is needed. Following EMPIRE philosophy, a file with collective levels is created in the first run and user may change default model parameters in subsequent runs.

CSISRS/EXFOR database

The FORTRAN based retrieval of experimental data used in the previous versions of the code has been replaced by a Java software interacting with the relational database (MySQL). While the convenient feature of the transparent retrieval during the EMPIRE run is preserved, the new software also enables arbitrary queries through the powerful graphic interface (essentially identical to the web version). The main advantage of the new approach is that EMPIRE will be able to use the most recent version of the EXFOR library periodically issued (CD-ROM) by the IAEA.

CONCLUSIONS

The 2.19 release of the EMPIRE code adds most of the functionalities of practical importance that were missing in the 2.18 version. The extension of the fission channel allows to treat the most complex cases including low energy neutron induced fission on actinides with multiple-humped fission barriers. Preequilibrium emission of clusters can be handled within the Iwamoto-Harada model providing for a physically sound description of α and deuteron spectra. All photon channels are formatted allowing for a complete γ-ray production being included in the ENDF file. Capability of treating photon induced reactions as well as reactions on excited targets allows EMPIRE to embrace new types of reactions of interest for certain applications.

Further development will address Hauser-Feshbach calculations of prompt fission spectra, capability of estimating covariances and even closer integration with the new library of input parameters (RIPL-3).

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