Status Report on the WPEC / Subgroup A Activities in 2004-2005

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Abstract:
The primary goal of the long-term Subgroup A is to promote collaboration and exchange among nuclear reaction code developers internationally. This document reports on the Subgroup A activities in 2004-2005, both in view of individual codes (TALYS, EMPIRE, GNASH/McGNASH) development, and in regard to the common development of the ModLib library. Notably, several important new code releases were made this year: the TALYS code v.0.64 was released in January 2005; a new and significant update of the EMPIRE code (v.2.19) was released in late March 2005; and the first version (v.0.1) of the ModLib library was also released in December 2004. Finally, the McGNASH code is still in development at LANL and a beta-version is expected to be released by the end of 2005.

1 Status of existing nuclear reaction codes

1.1 EMPIRE-2.19, Lodi

Lot of work has been invested over last two years into improvement and adding new functionalities to the EMPIRE code. Extensive testing has been carried out recently leading to the beta version (EMPIRE-2.19, Lodi), released by the end of March 2005. It includes following new features and improvements:

- 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.

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.

Encouraging results 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 [**?**]. In this model, the formation probability of a cluster takes into account excitons below and above the Fermi surface and avoids free parameters.

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), (iii) Generalized Fermi Liquid model (GFL), and (iv) three versions (MLO1, MLO2, and MLO3) of the Modified Lorentzian model by Plujko 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 photo-absorption 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 standard Hauser-Feshbach model.

Exclusive spectra

For the 2.19 version of the code a completely new approach, based on the concept of the 'population spectra', has been developed. 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.

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)

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.

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).

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).

1.2 TALYS-0.64

GENERAL

TALYS, written by A.J. Koning, S. Hilaire, and M.C. Duijvestijn, is a computer code system for the prediction and analysis of nuclear reactions, created at NRG Petten, the Netherlands and

CEA Bruyeres-le-Chatel, France. The basic objective behind the construction of TALYS is the simulation of nuclear reactions that involve neutrons, gamma-rays, protons, deuterons, tritons, He-3 and alpha-particles, in the 1 keV - 200 MeV energy range With the TALYS code system we aim to cover the whole path from fundamental nuclear reaction models to the creation of complete data libraries for nuclear applications. To achieve this, we have implemented a suite of nuclear reaction models into a single code system. This enables us to evaluate nuclear reactions from the unresolved resonance region up to intermediate energies. TALYS can be used for the analysis of experiments for basic scientific purposes or to generate nuclear data files. An additional long-term aim is full transparency of the implemented nuclear models, in other words, an understandable source program, and a complete modular structure.

We divide this short report in four parts: Release, features of TALYS, specific additions in 2004-2005, and features under construction. The code has been used for various publications, and we therefore include a reference list of publications from 2004 onwards. At the moment, the official TALYS reference is:

A.J. Koning, S. Hilaire and M.C. Duijvestijn, “TALYS: Comprehensive nuclear reaction modeling”, Proceedings of the International Conference on Nuclear Data for Science and Technology - ND2004, Sep. 26 - Oct. 1, 2004, Santa Fe, USA.

RELEASE

The first beta version that has been released to the public is TALYS-0.64. The release was announced at the ND-2004 conference in Santa Fe and was delayed to December 5 2004. There are currently 75 persons that have shown interest and have received the code.

A lot of effort has been put in completing the manual and constructing a large set of sample cases that covers most of the code’s capabilities.

FEATURES

- In general, a non-approximative implementation of many of the latest nuclear models for direct, compound, pre-equilibrium and fission reactions.
- A continuous, smooth description of reaction mechanisms over a wide energy range (0.001-200 MeV) and mass range ($5 < A < 339$).
- Completely integrated optical model and coupled-channels calculations through the ECIS code.
- Incorporation of new optical model parameterisations for many nuclei.
- Total and partial cross sections, energy spectra, angular distributions, double-differential spectra and recoils.
- Discrete and continuum photon production cross sections.
- Excitation functions for residual nuclide production, including isomeric cross sections.

- Automatic reference to nuclear structure parameters as masses, discrete levels, resonances, level density parameters, deformation parameters, fission barrier and gamma-ray parameters, generally from the IAEA Reference Input Parameter Library.
- Various width fluctuation models for binary compound reactions and, at higher energies, multiple Hauser-Feshbach emission until all reaction channels are closed.
- Various phenomenological and microscopic level density models.
- Various fission models.
- Models for pre-equilibrium reactions, and multiple pre-equilibrium reactions up to any order.
- An exact modeling of exclusive channel cross sections (e.g. (n,2np)), spectra, and recoils.
- Use of systematics if an adequate theory for a particular reaction mechanism is not yet available or implemented, or simply as a predictive alternative for more physical nuclear models.
- Automatic generation of nuclear data in ENDF-6 format. (commercial release only)
- A transparent source program.
- Input/output communication that is easy to use and understand.
- An extensive user manual.
- A large collection of sample cases.

FEATURES ADDED IN 2004-2005

- Release/publication of the code: 1. Manual completed: 297 pages 2. A large number of sample cases covering various different nuclear reaction types
- Construction of the code TASMAN, for two purposes: (a) automatic fitting of any partial cross section to the experimental data, for only one channel up to many channels and nuclides simultaneously, (b) covariances produced by Monte Carlo sampling of the input parameters. Also a full sensitivity matrix for the input (nuclear model) parameters of TALYS can be obtained. TASMAN is a code built around TALYS (TALYS is called by a system() function). TASMAN is not freely available.
- Complete ENDF-6 format generator, called TEFAL, enabling to use the most modern procedures for ENDF-6 files with MF1/2/3/4/6/8/10/33. Full description of energy-angle distributions, discrete and continuum photon production, etc. for all exclusive pathways. Only missing item is recoils. Also, activation cross sections for non-threshold reactions can now be stored in MF9. The addition compared to last year is MF33 for covariances. TEFAL is not freely available.

- An exact and a more approximative model for recoils. The latter is now somewhat more suitable for ”practical” calculations, though still not ideal. Also, a simple binary CM-to-LAB conversion option was added.
- Revision of the fission model, especially by including more flexibility of damping of shell and collective effects for fission level densities.
- Extension of scripts to run TALYS for mass production of nuclear data.

UNDER CONSTRUCTION

- Official release version 1.0, incorporating findings by the current set of beta testers.
- Addition of optimization, sensitivity matrices, and covariance generation for angular distributions, spectra and gamma-ray production cross sections to the TASMAN code (right now, this only covers cross sections).
- Addition of MF34 (covariances for angular distributions) to TEFAL code.
- Revision of complex particle emission model using new publication by Kalbach.
- Automatic fission calculations, i.e. improvement of ”zero-order” answers, through a better calibrated fission database.
- Improvement of modularity.

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1.3 McGNASH

The McGNASH code is written at Los Alamos by P. Talou, M.B. Chadwick, T. Kawano and P.G. Young. It is a modern version of the well known GNASH code written by P.G. Young, M.B. Chadwick and E.D. Arthur. Its purpose is very similar to the one of EMPIRE or TALYS.

McGNASH is not yet available for public release, but a beta-version of the code is expected to be released internally by the end of 2005.

McGNASH incorporates most features already present in the set of codes GNASH, GSCAN and RECOIL, all part of the LANL suite of codes used to generate ENDF evaluated nuclear data files.

Features of the McGNASH code now include:

- Full implementation of the Hauser-Feshbach (HF) decay of a compound nucleus through multiple emission of n,p,d,t,h,α particles;
- Link to the ECIS03 coupled-channels code by J. Raynal (CEA) to compute direct reactions and transmission coefficients used in the subsequent HF equations;
- Implementation of the Ignatyuk-Gilbert-Cameron prescription for defining level densities;
- Kopecky-Uhl gamma-ray strength function formalism;
- Fission model similar to GNASH's original double-humped barrier;
- Width Fluctuation corrections (GOE, HRTW and Moldauer);
- Inclusion of the DDHMS module to compute pre-equilibrium emission and spin transfers;
- Exact calculation of exclusive spectra;
- Automatic link to the RIPL-2 database of parameters for default calculations;
- Automatic plotting capabilities with the GNUPLOT free software (cross sections, individual and composite spectra, etc);
- Development of a Suite of sample cases;
- Easy/natural link to the ModLib library modules.

McGNASH is written in modern Fortran 95 language, and makes an extensive use of the capabilities of this language in order to render the code clear and easily upgradable. McGNASH is a set of F95 modules that are well encapsulated and as much independent from each other as possible. During its development, McGNASH is being constantly benchmarked against GNASH. It also uses a suite of test cases in order to fully test each feature of the code.

The input file is much simpler and intuitive than GNASH's input file, and in the simplest case, is reduced to only a few lines, most parameters being taken from a database for default values.

To be added in the near future:

- photo-nuclear reactions;
- Improvement of the fission model;
- Link to a Monte Carlo module to treat the de-excitation of fission fragments by neutron and gamma emissions;
- Automatic ENDF formatting for all physical quantities calculated in McGNASH;
- Generation of covariance matrices with the KALMAN code (T.Kawano);
- Extension of the manual / web.

2 Modlib-0.1

The Modlib library is a set of Fortran 95 modules that can be used in existing and future nuclear reaction codes to treat different parts of nuclear reaction mechanisms and nuclear structure. Because of its standardized form, a Modlib module can easily be integrated in any nuclear reaction code (e.g., EMPIRE, TALYS or McGNASH) and be used to test, replace or add a particular capability.

Codes inter-comparison would be greatly facilitated through the use of the library, since entire portions of the different codes could be easily replaced by Modlib modules, and then sample cases tested with more or less modules included.

The Modlib project is the result of the work of the Subgroup A participants. In particular, A.J. Koning, M. Herman, C. Dunford and P. Talou have been the main actors so far.

The first version of Modlib, version 0.1, was released in December 2004, and was sent to the NEA databank in Paris for official release. A web site will also be set up to facilitate the distribution of the library, and the communication among developers and users.

This first version is composed of a set of physics modules that include the calculation of: Ignatyuk-Gilbert-Cameron level density formalism, gamma-ray strength function formalism, and width fluctuation corrections (three approaches). All physics constants used in Modlib are taken from the official ENDF values, as referenced in the ENDF-102 manual (Ed. V.McLane, 2001). The latest versions (in Fortran 90) of the ENDF checking and formatting codes STANEF, CHECKR, FIZCON, and PSYCHE, written by C.Dunford (BNL), were also included as modules in the library.

Developers of Modlib are also involved in the IAEA/CRP on RIPL-3. A natural link between Modlib and RIPL3 is being worked out through the development of nuclear reaction parameters retrieval codes.

In the coming year, Subgroup A members will work on two main tasks:

- Use and test Modlib-0.1 in EMPIRE, TALYS and McGNASH;
- Develop new modules for Modlib-0.2.

The first task will be to ensure that Modlib modules can be easily incorporated into the main three reaction codes in use at present. This is a particularly important step for the further acceptance and development of the library.

In regard to the modules being thought after for Modlib-0.2, LANL is proposing to distribute the pre-equilibrium DDHMS code as a Fortran 95 module. M.Herman has proposed to include the EMPIRE-specific level densities into the next version of Modlib. Choices on other modules will also be decided during our April 2005 meeting in Antwerp.

In addition, RIPL-3 members will be working on modules to provide a natural interface to the RIPL database. All RIPL3 modules will be included in the next version of Modlib.