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Title: Subgroup A: Nuclear Model Codes Report to the Sixteenth Meeting of the WPEC

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Subgroup A: Nuclear Model Codes
Report to the Sixteenth Meeting of the WPEC Aix-en-Provence, France, May 26-28, 2004

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Executive Summary

The Subgroup A activities focus on the development of nuclear reaction models and codes, used in evaluation work for nuclear reactions from the unresolved energy region up to the pion threshold production limit, and for target nuclides from the low teens and heavier. Much of the efforts are devoted by each participant to the continuing development of their own Institution codes. Progresses in this arena are reported in detail for each code in the present document. EMPIRE-II is of public access. The release of the TALYS code has been announced for the ND2004 Conference in Santa Fe, NM, October 2004. McGNASH is still under development and is not expected to be released in the very near future. In addition, Subgroup A members have demonstrated a growing interest in working on common modeling and codes capabilities, which would significantly reduce the amount of duplicate work, help manage efficiently the growing lines of existing codes, and render codes inter-comparison much easier. A recent and important activity of the Subgroup A has therefore been to develop the framework and the first bricks of the ModLib library, which is constituted of mostly independent pieces of codes written in Fortran 90 (and above) to be used in existing and future nuclear reaction codes. Significant progresses in the development of ModLib have been made during the past year. Several physics modules have been added to the library, and a few more have been planned in detail for the coming year.

Detailed Report

This document is organized as follows: Part-I is devoted to the description of each individual nuclear reaction code, its status, recent additions, and future developments. Part-II describes the status of the ModLib library.

PART-I: Status of Existing Nuclear Reaction Codes

1. EMPIRE

Recent Developments of the Nuclear Reaction Model Code Empire

M. Herman, R. Capote, P.Oblozinsky, M. Sin, A. Trkov, A. Ventura
V. Zerkin

EMPIRE-II is a system of codes 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 design 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 available experimental data can be obtained with just a few mouse clicks and key strokes.

Empire-II includes most of major nuclear reaction mechanisms, such as spherical optical model (SCAT2) and Coupled Channels (ECIS), Multi-step Direct (ORION + TRISTAN), NVWY Multi-step Compound, exciton model (DEGAS), Monte Carlo preequilibrium emission, and the full featured Hauser-Feshbach model with width fluctuation correction (HRTW). A comprehensive library of input parameters, based on RIPL-2, covers nuclear masses, optical model parameters, ground state deformations, discrete levels and decay schemes, level densities, fission barriers (BARFIT), moments of inertia (MOMFIT), and gamma-ray strength functions. The results can be converted into the ENDF-6 format using the accompanying code EMPEND. 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.

In the present contribution recent developments, extending functionality and applicability of the system will be discussed. These include: (i) new algorithm for disentangling emission spectra into exclusive components, (ii) treatment of the recoils spectra, (iii) state of the art handling of the fission channel through the multiple fission barrier, (iv) merging resonance region into the final evaluation, (v) extended formatting and plotting capabilities, and (vi) new user graphic interface.

In addition: (i) new exciton model with cluster emission using Iwamoto-Harada approach, (ii) photo-nuclear reactions, (iii) six approaches for the gamma-strength function (RIPL-2).

2. McGNASH

McGNASH is being developed in Los Alamos and aims at replacing the GNASH code. It is written in modern Fortran 95, and makes a large and consistent use of Fortran modules.

About 20 modules have now been written and cover a large set of features required in a modern "state-of-the-art" nuclear reaction code.

Last year, the DDHMS pre-equilibrium code by M.B. Chadwick written in F77 was modified and encapsulated in a F95 module. This code performs Monte-Carlo simulations of the pre-equilibrium phase using the Hybrid model developed by M. Blann.

The fission channel has also been included. So far, it follows closely the simple double-humped barrier with uncoupled oscillators approach implemented in the GNASH code. However, we expect to include the recent work by E. Lynn on width fluctuations in the two wells in the near future. Also, we intend to make use of the five-dimensional calculations by P. Möller in order to allow for multi-paths fission.

An option for calculating exclusive spectra (as opposed to the "standard" inclusive) has also been implemented, but remains to be tested. This is will be done in collaboration with members of the LANSCE facility in Los Alamos, and in conjuction with some experiments which do require exclusive spectra calculations for comparison.

Finally, the manual is growing along with the code. It is organized following the modular structure of the code, and for each module, contains explanations about the functionalities and the use of the module and routines therein. In addition, a suite of test cases is being developed with the goal of testing each particular facet of a nuclear reaction calculation.

3. TALYS

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 and for target nuclides of mass 5 and heavier. 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 for applications.

The development of TALYS follows the "first completeness, then quality" principle, i.e. we aim to enhance the quality of TALYS equally over the whole reaction range and always search for the largest shortcoming that remains after the last improvement. The reward of this approach would eventually be that with TALYS we can cover the whole path from fundamental nuclear reaction models to the creation of complete data libraries for nuclear applications. 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.

The current version is TALYS-0.58. It is not generally available, but we expect to release TALYS at the ND-2004 conference in Santa Fe.

We divide this short report in three parts: General features of TALYS, specific additions in 2002-2003, and features under construction.
Also, the code is now coming to surface in various publications, although we still need to produce the official TALYS publication, and we therefore include a reference list here.

GENERAL 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 2003-2004

- The two-component exciton model has been refined and extended up to any order in multiple pre-equilibrium emission. Also, a numerical implementation of the reaction dynamics has been realized (in addition to the existing analytical solution), enabling more general nuclear structure inputs (such as microscopic particle-hole densities) and an exact computation of the exciton model equations. A new systematical relationship for the neutron-proton dependent matrix element has been found, which enables a proper pre-equilibrium description for 7 < E < 200 MeV. Also, an exciton model directly based on the optical model has been implemented, making the model more parameter free.
- Complete ENDF-6 format generator, enabling to use the modern (Los Alamos based) format for ENDF-6 files with MF1/2/3/4/6/8/10. 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.
- An exact and a more approximative model for recoils. The latter is now

somewhat more suitable for "practical" calculations, though still not ideal.
- Automatic coupled-channels calculations with the rotational, vibrational, rotational/vibrational, and asymmetric rotational model.
- Extension of fission model to higher energies (multi-chance fission from any residual nucleus bin). Prediction of fission fragment distribution with the Brosa model at all (low and high) energies. Flexibility of damping of shell and collective effects for fission level densities.
- Dispersive neutron optical models for all non-deformed nuclei.
- Possibility to read in parts of existing ENDF-6 data libraries, both resonances and total cross sections, to be merged with TALYS-produced results.
- Reliable estimates for non-threshold reactions (n,gamma), (n,alpha), (n,p) down to thermal energies using extrapolation and thermal experimental data. This is done in collaboration with J. Kopecky.
- Scripts to run TALYS from dripline to dripline, and to produce data for activation files such as EAF.

UNDER CONSTRUCTION

- An approximative model for recoils ("Chadwick" model), enabling mass production of recoil information within a reasonable timescale.
- Automatic fission calculations, i.e. improvement of "zero-order" answers, through a better calibrated fission database.
- Improvement of modularity, transfer to Fortran 90.
- The final manual, and an official publication of the code.

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4. COH

COH is a nuclear reaction code developed by T.Kawano (LANL) and written in C and Perl. The following lines provide a snapshot on the existing (stable) version characteristics and on the ones of the upcoming alpha-version:

Current stable version - 2.2 (denoted by +)
Experimental version - 3.0 alpha (denoted by -)

+ Coupled-Channels Calculations are available for the entrance channel
  + Rotational model, mainly for actinides
  - Full-coupling of CC and HF
  - Kawai-Kerman-McVoy theory calculation

- Fission calculation
  - Transmission of fission channles by P.Moller's potential calculation

+ Perl program, ripl2coh
  + generates CoH input file from the RIPL-2 library
  - new level density parameter systematics with P.Moller's shell/pairing energies

Part-II: ModLib

A Library of Fortran Modules for Nuclear Reaction Codes

ModLib is a library of Fortran (90-compatible) modules to be used in existing and future nuclear reaction codes. The aim is to constitute a library of well-tested and well-documented pieces of codes that can be used with confidence in all our coding efforts. This effort will undoubtedly help avoid the duplication of work, and most certainly facilitate the very important inter-comparisons between existing codes.

The modules are written in modern Fortran 90/95 scientific language, which represents a major leap from older Fortran 77 coding style and possibilities. A major emphasis is made on the reliability and the capacities of evolution of these modules. In other words, it is of fundamental importance that these modules be written in a way that they can be easily understood and eventually modified/upgraded later on, when/if errors are found or physics models improved.

Along these lines, a system of license numbering has been put in place. Also, a set of coding, documenting and testing rules have been agreed upon.

Here is the list of modules developed so far:

- WIDTH_FLUCTUATIONS [Talou, Chadwick]: calculates width fluctuation correction factors (output) for a set of transmission coefficients (input). Three methods are available: HRTW, Moldauer, and Verbaarschot (also called GOE approach). So far, no distinction is made according to the type of the coefficients channels (particle emission, gamma-ray emission, fission).

- GAMMA_STRENGTH [Herman]: calculates gamma-ray transmission coefficients using a Giant Resonance formalism.

- LEVEL_DENSITY [Koning]: computes the Gilbert-Cameron-Ignatyuk formalism for the continuum nuclear level density.

- CHECKR, FIZCON, INTER, PSYCHE, STANEF [Dunford]: these processing codes are already well known and commonly used by most ENDF evaluators. Originally written in Fortran77, they have been entirely re-written as Fortran90 modules following ModLib coding and submission rules.

- DDHMS [Chadwick, Talou] - *to be submitted*. The preequilibrium DDHMS.F code originally written in Fortran77 has also been partly re-written in modern Fortran90, and should be submitted shortly as an additional module to the ModLib library.

Another important module concerns a set of numerical routines commonly used in a nuclear reaction code. While trying not to re-invent the wheel, we are however bound by copyright infringement issues (e.g., the use of routines from Numerical Recipes™ within ModLib is not a good idea). There exists however the GSL or "GNU Scientific Library" (http://www.gnu.org/software/gsl/) that is free software under the General Public License. Although written for C and C++ programmers, it might be possible to adapt it to our present needs at small expenses. Efforts in this direction will be investigated.

Extensions of the existing modules or/and development of new modules will also be discussed at the occasion of the May 25 meeting.

The ModLib website (http://www.nndc.bnl.gov/nndcscr/model-codes/modlibs/) is being re-written in order to better fit the present needs. Particular additions or/and modifications will be discussed during our May 25 meeting.

Again, to help organize this international effort, two mailing lists exist: one whose goal is to discuss technical details and very preliminary modules among developers (modlib-dev@lanl.gov) and the other one, more general, intended for modules releases and other important announcements (modlib@lanl.gov). To subscribe to these lists, please just send an email to listmanager@lanl.gov, with the following line in the body of the message: "subscribe modlib@lanl.gov" or "subscribe modlib-dev@lanl.gov", for the general and the developers lists, respectively.