

## **Subgroup A: Nuclear Model Codes**

### **Report to the WPEC Meeting, San Diego, May 13-15, 2003**

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#### **Abstract**

In this report, last year activities of the Subgroup A are summarized, and organized in two distinctive parts: (1) Current status of the main existing nuclear reaction codes; (2) Progress report on the library of nuclear reaction modules. This paper also discusses the topics to be addressed during the latest Subgroup A workshop held just prior to the San Diego meeting.

#### **Status of Existing Nuclear Reaction Codes**

##### **1. EMPIRE**

Development of the EMPIRE-II code continued over the last year resulting in the release of the 2.18 (Mondovi) version in October 2002. Apart of bug fixes and minor changes, the main improvements were:

1. Formating of gamma-branching ratios in the ENDF file (A. Trkov).
2. Gamma-strength function uses a temperature consistent with the current level densities for the final state (M. Herman).
3. New Graphic User Interface (M. Herman).
4. PLOT4 updated to produce gamma-spectra (A. Trkov).
5. All collective levels (including closed channels) used in ECIS calculations. In the previous versions only open channels were considered and coupling to the closed ones was ignored (R. Capote).
6. Discrete level library updated to the RIPL-2 version as of September 24, 2002 (M. Herman).

Improvement of user friendliness with the new GUI is the most striking feature of this release. In particular, ZVView plotting capabilities were substantially extended by adding multiple double-differential plots for all ejectiles including gammas.

Subsequent development lead to the break-through in the treatment of the fission channel. Subbarrier fission through the triple-hump barrier is now possible due to the coordinated effort of R. Capote (Sevilla), M. Herman (Vienna/Brookhaven), M. Sin (Bucharest), and A. Ventura (Bologna), although width fluctuation correction should still be added to the formalism. Current (not released) version 2.19beta (Lodi) includes in addition:

1. Internal conversion coefficients in the gamma-cascade between discrete levels (ICC data from RIPL-2) (M. Herman)
2. ENDRES code and BNL-325 file with resonance parameters in order to merge resonance parameters into the final ENDF file (A. Trkov).
3. LINEAR and RECENT utility codes to reconstruct cross sections from the resonance parameters and enable plotting (M. Herman).
4. Option for manual fitting of Optical Model Parameters added to the new GUI (M.

Herman).  
5.PSYCHE and CHECKR added to the chain of utility codes (M. Herman).

These developments follow a general line of constructing a package capable of producing a complete and verified ENDF-6 file.

## 2. MCGNASH

MCGNASH is being developed in modern Fortran 95, and uses a very modular approach to treat the various parts of a nuclear reaction code.

Some “elementary bricks” modules have been written to defined basic information useful in the rest of the code:

- 1.Accuracy: this module defines the accuracy in which variables are declared and calculations performed.
- 2.Mainio: defines the main input/output file units.
- 3.Util: provides error/warning routines.
- 4.Physics: contains the definitions/values of various physics constants, as taken from the ENDF manual.

Two other modules can be considered as “basic” since they contain the definitions, and sometimes values, of global objects:

- ⑩Definitions: declarations of new objects (e.g., nucleus) to be used in the rest of the code.
- ⑩Database: includes all global variables/arrays/objects which are used in many parts of the code (replaces the use of COMMON block in F77).

The values of certain global objects are not necessarily given in these modules, but instead obtained (either calculated or read-in) within other modules.

There is also a couple of modules for input reading and output writing of information;

- ⑩read\_inputs: this module provides the routines used to read in data from various input files: main input file where the reaction to be studied is described (including the choices of physics models available), nuclear masses data file, transmission coefficients file (usually obtained using an optical model code such as ECIS), etc.
- ⑩results: it contains routines to output the results in a formatted way. So far, the formats used correspond to the ones developed earlier in GNASH itself.

Another module is also thought to directly format MCGNASH results into ENDF/B format. This will allow a very fast production mode for the release of new reactions evaluations.

The various physics modules which constitute the important part of MCGNASH have also been written:

- 1.Compound: this module provides many of the most important routines of the code: create\_nucleus, populate\_nucleus, decay\_nucleus, ... These routines usually rely on other physics routines present in other modules (such as fluctuations or level\_density).
- 2.Hauser\_feshbach: provides various routines to be used in compound, especially regarding the calculation of g-rays transmission coefficients, and splining of transmission coefficients. This is a very generic module which will eventually be replaced by several more specialized modules.
- 3.Level\_density: it provides the tools necessary to compute the nuclear level density

distributions in the continuum. So far, the user has the choice among three models as described in the PHYSICS part of this document.

4. Fluctuations: allows the computation of the width fluctuation correction factors, important at low-incident energies, where the pure HF result breaks down because of correlations in the elastic channel. Note that this module was provided to the general nuclear reaction community through the MODLIB International Collaboration effort (see below).

Finally, the main module is called "mcgnash" and implements the organigram used to perform an actual nuclear reaction cross section calculation: it first calls the input data entered by the user, then defines the chain reaction to be studied, follows the decay paths, and then finally calls routines to output the results in a human-readable way.

The writing of the MCGNASH manual is also in progress. It is basically split into two parts: the first one describing the physics implemented in the code and focussing on the parts relevant to its particular coding in MCGNASH, and the second part describing in detail the coding behind each Fortran module. This manual will be constantly updated following the coding of each new module.

In the near future, the code will be developed further to encompass the following three items:

1. Inclusion of the DDHMS preequilibrium code (Chadwick) into MCGNASH.
2. Treat the fission channel within the double-humped fission barriers model.
3. Implement calculation of exclusive spectra.

### 3. TALYS

TALYS, written by A.J. Koning and S. Hilaire, is a nuclear reaction program created at NRG Petten, The Netherlands and CEA Bruyeres-le-Chatel, France. TALYS is a computer code system for the prediction and analysis of nuclear reactions. The basic objective behind the construction of TALYS is the simulation of nuclear reactions that involve neutrons, photons, protons, deuterons, tritons, He-3 and alpha-particles, in the 1 keV - 200 MeV energy range and for target nuclides of mass 12 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.

The development of TALYS follows the "first completeness, then quality" principle. This should certainly not suggest that we use toy models to arrive at some quick and dirty results. On the contrary, several reaction mechanisms coded in TALYS are based on theoretical models whose implementation is only possible with the current-day computer power. It rather means that, in our quest for completeness, we try to divide our effort equally among all nuclear reaction types. The precise description of all possible reaction channels in a single calculation is such an enormous task that we have chosen not, to put it bluntly, to devote several years to the theoretical research and absolutely perfect implementation of one particular reaction channel which accounts for only a few millibarns of the total reaction cross section. Instead, 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.

TALYS is not yet generally available.

We divide this short report in three parts: General features of TALYS, specific additions in 2002-2003, and features under construction.

### **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 ( $12 < A < 339$ ).
- Completely integrated optical model and coupled-channels calculations through the ECIS code.
- Incorporation of new optical model parameterizations for many nuclei.
- Total and partial cross sections, energy spectra, angular distributions and double-differential spectra.
- 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 RIPL-database.
- Various width fluctuation models (Moldauer, HRTW and GOE) for binary compound reactions, and multiple compound emission (Hauser-Feshbach) until all reaction channels are closed.
- Various phenomenological and microscopical level density models.
- Classical (exciton model) and quantum-mechanical (multi-step direct, FKK) models for pre-equilibrium reactions.
- An exact modelling of exclusive channel cross sections (e.g.  $(n,2np)$ ) and spectra.
- Use of systematics (e.g. Kalbach systematics) if an adequate theory for a particular reaction mechanism is not yet available or implemented, or simply as a predictive alternative for the nuclear models in TALYS.
- Automatic generation of nuclear data in ENDF-6 format.
- Transparent programming.
- Input/output communication that is easy to use and understand.
- An extensive user manual.
- A large collection of sample cases.

### **Additions in 2002-2003**

- The two-component exciton model has been refined and extended up to any order in multiple pre-equilibrium emission. A new systematical relationship for the neutron-proton dependent matrix element has been found, which enables a proper pre-equilibrium description for  $10 < E < 250$  MeV.
- Kalbach's latest complex particle emission model (C. Kalbach, to be published) has been adapted from PRECO-2000 and tested successfully against data, including the new (n,xp....xa) measurements from the HINDAS project.
- 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, due to time limitations, see below.
- Photon-induced reactions.
- Possibility to evaluate reactions on isomeric targets.
- Systematics for reaction cross sections for all particles (Tripathi model).
- More choices for fission barriers (Sierk, RLDM, Maslov).
- Automatic calculations for natural targets.
- Giant resonance contribution to the continuum.
- An exact model for recoils. (which, presently, is not suitable for "practical" calculations, see below.
- 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 optical models for all non-deformed nuclei.

### **Under construction**

- An approximative model for recoils, enabling mass production of recoil information within a reasonable timescale.
- Automatic fission calculations, i.e. improvement of "zero-order" answers.
- Improvement of modularity, transfer to Fortran 90.
- Possibility to read in parts of existing ENDF-6 data libraries, to be merged with TALYS-produced results.
- Automatic coupled-channels calculations with the rotational, vibrational, rotational/vibrational, and asymmetric rotational model.
- Transfer of FKK model for microscopic form factors from existing MINGUS code.

## **4. MOARC**

Improvements from last year's status:

We have made a GUI using Python and the Tkinter interface to tk/tcl, and have tested it on Windows and Linux platforms. This interface prepares the input file for the C++ Hauser-Feshbach program and executes it.

## **Library of Fortran Modules**

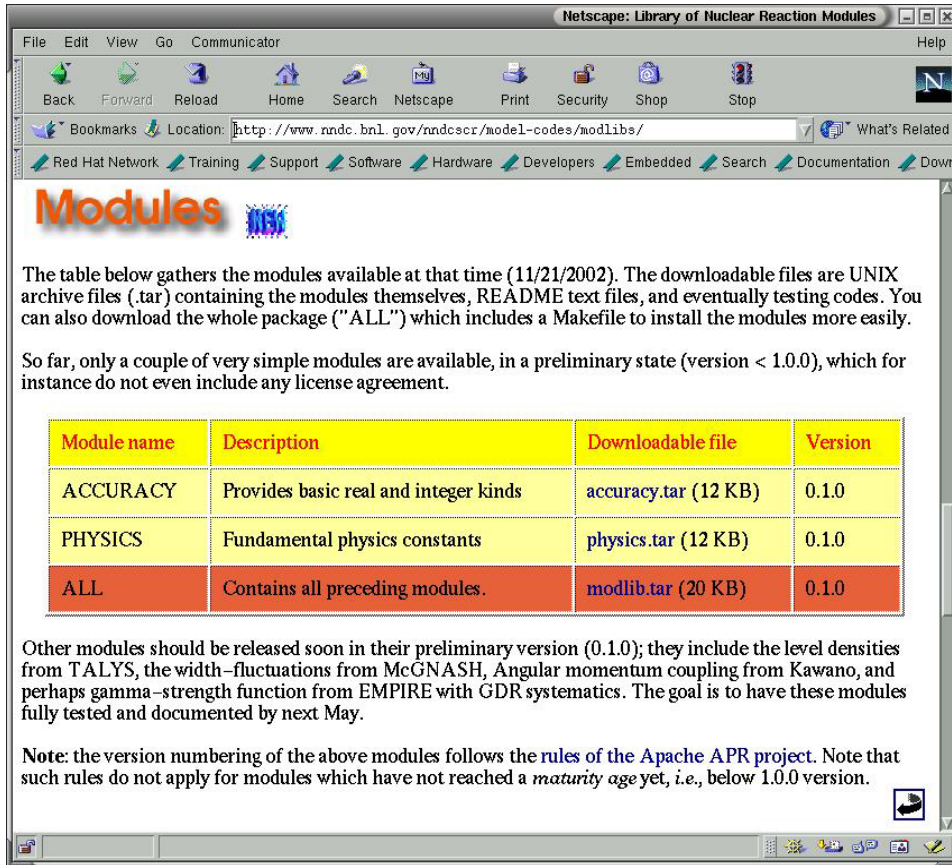
In the two last meetings of the Subgroup A, the important need for the development of a set of modern computer modules to be used in existing and future nuclear reaction codes was recognized, and the project was started. Such modules will eventually constitute a library of well tested and well documented pieces of codes which can be used safely and efficiently in all future programming efforts of nuclear reaction calculations. This effort will help avoid duplicacy work, and most certainly facilitate the very important intercomparisons between existing codes.

It was decided that this set of modules will be written in modern Fortran 90/95 scientific language, allowing the use of the best features of modern computer languages (modularity, encapsulation, etc). A particular emphasis is made on the reliability and evolutivity of these modules. In other words, it is of fundamental importance to write these modules in such a way they can be easily understood and eventually modified/upgraded later on, when/if errors are found or physics models improved. Therefore, a system of license numbering will be put in place. Also, a set of coding, documenting, and testing rules will be discussed during our May 12<sup>th</sup>, 2003 meeting. This will ensure a fair level of quality assurance.

The main developers of existing nuclear reaction codes have agreed to each contribute to this international effort by providing some pieces of code. To this day, three modules are already being discussed among the main developers, and some beta-versions should be released in the near future. The exact way these modules will be provided will also be discussed at this meeting.

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

A web site has been created to help centralize the information. It is hosted by the NNDC at Brookhaven: <http://www.nndc.bnl.gov/nndcscr/model-codes/modlibs/>. Below is a screenshot of part of this web page showing the Modules section where the development of modules is described. Note that two new modules have already been submitted to the Developers list: level density (Koning) and width fluctuations (Talou). These are much more important and complex modules than the ones presented on the web site so far. Another module has been sent out by Kawano regarding angular momentum coupling, but for now it is written in the C language only, and will need some additional coding in order to incorporate it into the standard library. All these modules, in their preliminary version, will be discussed thoroughly at our next meeting.



The meeting in San Diego will be organized as follow: first, the current coding efforts will be presented and discussed. Second, the various rules for coding, documenting, testing, etc, the modules will be discussed and hopefully set. Finally, the participants, both developers and users, will decide upon a priority list for new modules to be written or/and current modules to be extended.

Once the initial rules are defined and the first modules firmly in place, one can expect to see the development of this library getting much faster and more efficient, and the library becoming a major and powerful tool for the future progress of nuclear reactions simulations.