

Subgroup A: Nuclear Model Codes

Mark Chadwick (LANL), Arjan Koning (Petten),
Pavel Oblozinsky (BNL), Mike Herman (Vienna), Frank Dietrich (LLNL)

Abstract

This report provides an overview of Subgroup A activities that have taken place in the last year, as well as providing a statement of our short-term and long-term goals, and connections to the IAEA RIPL project. It also discusses a workshop on nuclear reaction physics and codes that is being organized prior to the Santa Fe WPEC meeting.

Short-term goals

The Subgroup fosters close collaborations between researchers involved in some of the most important nuclear reaction codes used for nuclear data evaluation and for interpretation of physics experiments. Since a number of efforts to develop modern statistical model codes are underway, such collaborations and code inter-comparisons are extremely valuable. They allow code developers to take advantage of new developments by other researchers in Subgroup A. The principal researchers and codes participating in Subgroup A to date are: A. Koning and S. Hilaire (code TALYS), M. Herman (EMPIRE), P. Oblozinsky (EMPIRE and HMS), F. Dietrich (STAPRE and new LLNL code), and M. Chadwick (McGNASH and HMS).

Specific short-term goals of the Subgroup can be formulated as follows:

1. Design and exchange of modules. We have an emphasis on designing code modules in a modular fashion that can be used straightforwardly by other researchers. Examples are given in the detailed discussion below: (1) Groups using a new Hybrid Monte Carlo Simulation (code HMS) preequilibrium module in their respective codes; (2) Groups using an exciton preequilibrium module DEGAS; (3) Collaboration to exchange modules and physics of width fluctuation corrections and recoils; (4) Collaboration to use the deformed optical model and coupled-channels code ECIS as a standard module.

2. Inter-comparison of codes. Code inter-comparisons are valuable for validating and benchmarking new code and physics developments. Last year, new Hauser-Feshbach routines in McGNASH and TALYS were tested against each other. Additionally, successful intercomparisons were made between McGNASH, GNASH, and STAPRE (Chadwick and Dietrich). This same inter-comparison suggested errors in the IDA Reffo code used at Livermore.

3. Links to RIPL. The third short-term goal, already being realized, is the development of our reaction model codes to read directly input model parameters recommended and created by the IAEA RIPL project. Examples include an automated code produced at Los Alamos, based upon the ECIS optical model code, to read RIPL information on both spherical and

deformed optical models and generate the transmission coefficients and inelastic scattering cross sections needed by statistical model codes. In general the reaction codes GNASH, McGNASH, TALYS, EMPIRE, etc are being improved to be able to directly use the RIPL parameters.

Long-term goals

The Subgroup is considering two potential long-term goals. The first of them is viewed as a realistic, the second one most likely not.

1. To develop a set of well-documented and tested modules for the physics packages of importance in statistical nuclear reaction codes.

In the longer term, the Subgroup aims to develop a set of well-documented and tested modules for the physics packages of importance in statistical nuclear reaction codes. These modules could then, relatively easily, be incorporated into a researcher's model code as needed. We think this is a realistic goal. The HMS preequilibrium module that has already been produced, and distributed to the Subgroup participants, is an example of this. Future capabilities would include features such as modules for width-fluctuation physics, Hauser-Feshbach, level densities, fission decay, optical models *etc.* The IAEA has expressed an interest in this goal too, and IAEA support for this activity in the form of codes that utilize the RIPL model input data would provide useful additional support.

2. To develop an international code for nuclear data evaluation.

This, more ambitious long-term goal may face a number of difficulties. WPEC provides an umbrella organization to help stimulate collaborations, but provides no support for code development. Attempts to produce one international code may ultimately succeed, but would have to solve a major issue – such a code should be supported/maintained and it may be difficult to find a long-term person/team with the resources and motivation to maintain such a code. Individual scientists at different labs have a high-motivation to keep control over their individual codes, in order to have a solid understanding of the physics and algorithms used and to maintain local skills and capabilities. Such scientists are likely to find a set of modules to be most useful. How this issue develops in the coming years is unclear, and we are keeping an open mind as to the most effective directions the Subgroup can take.

Detailed discussion of activities during last year

Code inter-comparisons

In order to validate new code developments, inter-comparisons have taken place between Chadwick, Dietrich, and Koning to test our Hauser-Feshbach modules. As might be expected, this process took longer than at first anticipated since we had to ensure every input parameter was identical (nuclear levels and decay properties; level densities, spin cut-off parameters in the different level density regions; transmission coefficients; gamma-ray

multipolarities and strength functions, etc). After a week-long visit to LANL by Dietrich, we were able to establish exact agreement between McGNASH, GNASH, and STAPRE.

HMS

A HMS preequilibrium Monte Carlo module has been completed and distributed by Chadwick, together with test cases. This self-contained module can be incorporated into other statistical model reaction codes – indeed, Herman and Dietrich have been including this module into their respective codes. Oblozinsky visited LANL to collaborate on one aspect of this module prior to its release – a preequilibrium spin distribution model was developed to allow the code to be linked with Hauser-Feshbach codes. This is particularly important for modeling spin-dependent observables such as isomer production, and the production of characteristic gamma-rays in residual nuclei.

EMPIRE

The code Empire by M. Herman is an example of a modularized code. It is structured in a way suitable for adding complete modules that deal with specific aspects of nuclear reaction physics. After official release of Empire-2 in 2000, an extensive international collaboration was initiated to further improve the code, while still preserving its largely automated input parameter features. The objective was to meet specific requirements of nuclear reaction cross-section evaluators, mostly of the BNL-KAERI project on fission products.

Over the past year, the following improvements have been completed or are nearing completion:

- Width fluctuation correction. The motivation was to improve capture and elastic cross section calculations at low energies. The HRTW approach was added (M. Herman), it performs very well and it is now routinely used.
- Second chance preequilibrium emission. The motivation was to extend application of the TUL-MSD to energies above 50 MeV, of interest to ADS applications. The method by M. Chadwick was selected in view of its straightforward application and proven performance. It turned out the TUL-MSD itself needs improvements at high energies.
- Exciton model with spin conservation. The primary motivation was to handle direct-semidirect capture in the fast neutron energy range. The exciton model code DEGAS was selected in view of its performance, proved to be equivalent with the sophisticated D-SD model. This new module was added (P. Oblozinsky), its initial testing gives good results.
- Deformed optical potential and coupled-channels. The motivation was to improve evaluations of fission products in the mass range $A > 150$. The code ECIS was selected in view of its generally accepted top performance. This new extensive module was added (R. Capote, Habana/Seville), and it is currently being tested.
- Hybrid Monte Carlo. The primary motivation was to extend the incident energy range well above 20 MeV, of interest to ADS applications. The promising HMS approach was selected, also thanks to its recent improvement by inclusion angular momentum effects (LANL-BNL collaboration). This new module was added (M. Herman), it is currently being tested.

- Recoils. This is important at higher energies, primarily for ADS applications. This new feature was added (M. Herman), largely using the ideas of M. Chadwick ut taking into account correlations between recoil spectra and excitation energy of decaying nuclei. Performance is currently being tested.

TALYS

TALYS is a nuclear reaction program created at NRG Petten, The Netherlands and CEA Bruyeres-le-Chatel, France. The idea to make TALYS was born in 1998, when we decided to implement our combined knowledge of nuclear reactions into one single software package, with the aim to use it as a tool in both nuclear physics and nuclear data. The basic objective behind the construction of TALYS is the ability to give a complete description of nuclear reactions that involve neutrons, photons, protons, deuterons, tritons, Helium-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. TALYS can then 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. This means that we aim to enhance the quality of TALYS equally over the whole reaction range and always search for the largest shortcoming, that still remains after the last improvement. The reward of this approach would 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 complete modularity.

As specific features of TALYS we mention

- In general, a non-approximate 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 parameterization 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. These come mostly from RIPL.
- Various phenomenological and microscopical level density models.
- Classical (exciton model) and quantum-mechanical (multi-step direct/compound) models for pre-equilibrium reactions.
- An exact modelling of exclusive channel cross sections and spectra.

- 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 the nuclear models in TALYS.
- Automatic generation of nuclear data in ENDF-6 format.
- Transparent modular programming.
- An input/output communication that is easy to use and understand.
- An extensive user manual.
- A large collection of sample cases.

The central message is that we always provide a complete set of answers for a nuclear reaction, for all open channels and the associated integrated, single- and double-differential cross sections, as well as activation/residual-production and fission cross sections. Depending on the current status of nuclear reaction theory needed for a particular reaction channel, this is done by means of more or less sophisticated physical methods. With TALYS, a complete set of cross sections can already be obtained with minimal effort, through a four-line input file of the type:

```
projectile n  
element U  
mass 235  
energy 14.
```

which, if you are only interested in robustness, reasonable answers or mass production of nuclear data, will give you all you need. If you want to be more specific, you simply add some of the more than 100 keywords that can be specified in TALYS.

Santa Fe workshop

LANL is hosting a workshop on nuclear reaction physics and codes, April 10-11, 2001, prior to the WPEC meeting. Organizers are Chadwick, Oblozinsky, and Dietrich. This meeting will discuss our goals for physics improvements and code developments in the coming year, and brings together many of the leading experts in this field. An outcome of the meeting will be an identification of key areas that will benefit from collaborations between scientists attending the meeting.