

Status report for NEA/WPEC nuclear model code activity
M.B. Chadwick and A.J. Koning, May 5 2000.

Background

At the NEA planning meeting in September 1999, it was agreed to establish an activity in nuclear model code development to be managed directly by the Working Party.

This group of researchers working in this area plans, in the long term, to develop an internationally-used, robust, reaction code (with advanced physics packages, and modern coding practices), for use in nuclear data evaluation and physics research.

The aim is to develop a code analogous to NJOY's role in data processing, i.e. well tested, reliable, and usable by a wide community of people. It should be usable at different levels: a simple input using default options, ranging to complex inputs for control of advanced options.

The code structure should be based upon independent "modules", each designed to provide a well-defined set of results from the variables passed to it. This will facilitate reliable validation and testing. In addition to the main code, the project would lead to an archived collection of documented modules for researchers to use.

This project also overlaps strongly with the IAEA's Reference Input Parameter Library (RIPL) coordinated research project, which recommends input information for model calculations.

Researchers at many labs (LANL, LLNL, ECN, CEA, JAERI, Duke, etc.) are currently developing new reaction modeling codes to update and supersede previous widely-used versions. There is quite a lot of duplication of effort. Much of this duplication is healthy (competition, novel approaches, different physics assumptions and theories). However, collaborations under the NEA-umbrella is useful in the following areas:

- Exchange of ideas. Additionally, the various code authors tend to have their own particular expertises (e.g. level densities, preequilibrium, width-fluctuations, etc), and sharing of modules related to these expertises would be helpful.
- Validation/testing. Code intercomparisons provide an opportunity for testing the accuracy of independently-developed codes. The NEA has played an important role traditionally in such code intercomparisons. In this work, the emphasis would be primarily on validation of correct implementation of various theories/models.

Status of progress

- In 1999 an email distribution was made calling for input on a NEA-coordinated international effort, and feedback was received from a number of possible participants
- Through discussions, we have begun the process of establishing features of various new codes that may be of wide interest for participants and other researchers
- We have determined which aspects of the codes can benefit from code intercomparisons:
- Hauser-Feshbach single-nucleus decay probabilities (and width fluctuations)
- Hauser-Feshbach sequential decay probabilities
- Preequilibrium predictions of emission spectra, and residual nucleus energy and spin distributions (for exciton, hybrid, Monte Carlo hybrid, quantum, QMD, etc theories, and for multiple preequilibrium)

- Fission decay probabilities
- Level densities (total, partial, fission)
- Transmission coefficients
- Gamma-ray strength functions
- Direct reactions
- At LANL, significant progress has been made in developing a new and modern version of GNASH, known as McGNASH. The code is being written in a modular fashion, using Fortran90. Over 4000 lines have been written. Significant testing/validation has been accomplished, through checks against GNASH predictions. (This has also led to identifying and removing some approximations in GNASH too). In Hauser-Feshbach validation tests (we focused on 20 MeV n+58Ni, allowing n,p,d,t,alpha,gamma ejectiles in sequential decay processes), we find agreement with GNASH to the better-than 0.2% level.
- At LANL we have also completed a first version of a Hybrid Monte Carlo preequilibrium module. A collaboration with Oblozinsky at BNL has begun in this area.
- Very good progress has been made in collaborations between ECN and Bruyeres-le-Chatel (Koning-Hilaire) on the development/testing of a nuclear reaction code system TALYS.
- Through the WPEC project, we have initiated intercomparison tests between US and Europe codes, to check the validity of the Hauser-Feshbach implementations. We expect this first-round of Hauser-Feshbach tests, initially for just 1-particle emission, to be completed within a short time.
- Researchers in the US have met, in the context of the US Data Program, to discuss the development of nuclear model codes at Los Alamos, Livermore, Argonne, and North Carolina (Kalbach).