

The Nuclear Reaction Code McGNASH

P. Talou*, M.B. Chadwick*, P.G. Young* and T. Kawano*

**Los Alamos National Laboratory, Los Alamos, NM, 87545*

Abstract. McGNASH is a modern statistical/preequilibrium nuclear reaction code, being developed at Los Alamos, which can simulate neutron-, proton- and photon-induced reactions in the energy range from a few-keV to about 150 MeV. It is written in modern Fortran 95 scientific language, offering new capabilities both for the developer and the user. McGNASH is still in a development stage, and a first public release is planned for later in 2005.

INTRODUCTION

The statistical/pre-equilibrium nuclear reaction code GNASH [1] has been used successfully over the years to compute neutron-, proton- and photon-induced reactions cross sections on a variety of nuclei targets, and for incident particle energies from tens of keV up to 150-200 MeV. This code has been instrumental in producing numerous nuclear data evaluation files for various ENDF libraries around the World, and in particular the ENDF/B-VI and pre-ENDF/B-VII libraries in the US. More recently, GNASH was used extensively for the creation of the LA150 library [2], including data on neutron- and proton-induced reactions up to 150 MeV incident energy. We are now developing a modern version of the code, called McGNASH.

CODING DETAILS

Written in old FORTRAN¹, the GNASH code was born in the early seventies and was continuously improved since then to incorporate new physics models. However, in doing so, the structure of the code has become very complicated and somewhat cumbersome to upgrade or even simply maintain. The advent of the modern Fortran 90/95 scientific language has open the path toward modern and higher-level programming techniques² that can be implemented efficiently to create a modern and powerful version of the GNASH code.

McGNASH is being written in Fortran 95.

It uses the concept of modular programming extensively. In fact, the McGNASH code is really a collection of such Fortran modules, each dealing with a specific (and often independent) part of the nuclear reaction sequence calculation. These modules are always written with the ideas of robustness and capacity to evolve in mind. By robustness, we mean a code that can be used throughout many computer platforms without having to tweak the inner coding structure. By capacity to evolve, we mean a code that is not bound to the physics models available at the time of the first release, but instead that can easily incorporate new and improved physics models when they become available. Fortran 95 makes it very easy to upgrade the inner code without the need for the external user to adapt to the new coding. Both concepts of robustness and capacity to evolve are linked: the code needs to be robust against new developments during its evolution. Although coding in Fortran 90/95 is not a condition *per se* to achieve these requirements, it definitely simplifies the coding, present and future.

The modular structure of McGNASH allows the development of independent modules simultaneously, without losing in consistency among the different modules. However, some basic modules are shared by all others, and constitute a library of objects and routines that can be re-used at will. The coding in McGNASH is strongly influenced by the notion of object-oriented programming, though it does not make use of some specific characteristics of this type of programming.

McGNASH is also being written with the user in mind. While a default GNASH input can be cumbersome to read or/and build for the non-expert, a McGNASH input has been reduced to a very simple and compact form, which can be easily tuned to any user's needs. We hope that this move will encourage the broad use of McGNASH outside its developer base community. Of course, simplicity and compactness come at a price. The same

¹ The current version of GNASH is written in FORTRAN77.

² Of course, Fortran 90/95 is not the only programming language that offers such high-level coding techniques- let us just mention the C/C++ language, for instance.

parameters appearing explicitly in a GNASH input are now "hidden" as default parameters in a McGNASH calculation. For simple and default calculations (or for producing large amounts of data over a large portion of the nuclear landscape), this last solution is certainly the best. However, in case the physics at hand is only poorly known, a default calculation might easily lead to relatively wrong answers, which only an expert-eye can detect. Hence, a word of caution may be worth here.

In order to get default calculations running for the most common nuclear reaction data needs, it is necessary to provide the code with default input data (e.g., discrete level schemes, optical model parameters, etc). To do so, we have chosen to link the RIPL-2 database [3] directly to McGNASH, hence providing default data for many nuclei and nuclear reactions.

Also, the 1996 version of the ECIS coupled-channels code [4] is still used to provide McGNASH with the transmission coefficients used in the Hauser-Feshbach equations. ECIS96 also provides the total and reaction cross sections, along with inelastic scattering cross sections and angular distributions to excited discrete levels.

For evaluation work, performing a nuclear reaction calculation is just not enough. The extraction and formatting of the pertinent results in a ENDF-type file is required. To achieve this task, GNASH uses an auxiliary code called GSCAN, which needs to be ran independently of GNASH. With McGNASH, this feature will be automatically available.

Finally, McGNASH will be able to produce postscript-quality plots of most of the numerical results directly at the outset of the computational run. In addition to tables of numbers, figures can be very useful to detect rapidly any potential mistake that may have occurred during the run.

PHYSICS MODELS

The basic physics models that constitute the backbone of the GNASH code are also present in McGNASH. A neutron- or proton-induced reaction on a heavy target leads to the formation of a compound nucleus in equilibrium, which then decays by emitting gamma-rays, neutron or light-charged particles, until a stable ground- or isomeric-state is reached.

The assumption of the formation of a compound nucleus in statistical equilibrium is not quite correct, especially at high and low energies. At high energies, the probability for emitting high-energy particles or clusters before the equilibrium is reached is not negligible anymore, and a pre-equilibrium stage has to be taken into account. On the opposite energy scale, the Bohr hypothesis of independence of the entrance and exit channels

breaks down due to interferences in the elastic channel. Corrections to the statistical picture have to be added.

The statistical decay of the compound nucleus is being modeled by the Hauser-Feshbach equations, using transmission coefficients to represent the relative probabilities of decay in the various open channels. The transmission coefficients for the light particle emissions (n,p,d,t, α) are obtained from an optical model calculation, commonly using the 1996 version of the ECIS code [4] or/and the SCAT code [5]. Both codes produce spin-dependent transmission coefficients that get imported into McGNASH. Note that, mostly for historical and technological reasons, the GNASH code never used the angular momentum and spin dependent transmission coefficients $T(l, j)$, but rather collapsed them into $T(l)$ values. This limitation has now been lifted in McGNASH. However, in most physical situations, the effect is negligible. In addition to the transmission coefficients, an optical model calculation provides the total and reaction cross sections. Coupled-channels or DWBA calculations are used to obtain direct excitation cross sections (and angular distributions) to low-lying states.

In both GNASH and McGNASH, the gamma-ray transmission coefficients are obtained from the gamma-ray strength function formalism of Kopecky and Uhl [6], which is derived from a generalized-Lorentzian description of observed Giant-Dipole Resonances. At higher incident energies, a Direct-SemiDirect model can best describe the capture cross section. To this end, we envision to include the results from the DSD code by Kawano [7] into McGNASH. An example of a DSD calculation is shown in Figure 1 for the neutron-capture cross section on ^{89}Y .

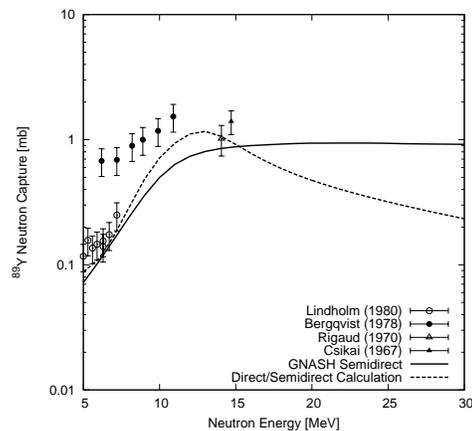


FIGURE 1. Neutron capture cross section on ^{89}Y : the role of the direct-semidirect process at higher energies.

The levels scheme representation in McGNASH is similar to the one in GNASH. The low-lying levels are read in from an external file (e.g., read from the RIPL-2 database) and matched to a density of states at higher-

energies. The description of the level densities $\rho(U, J, \pi)$ (where U is the excitation energy, J the spin and π the parity) in the continuum follows the Ignatyuk form of the Gilbert-Cameron formalism, including a washing-out of shell effects with increasing excitation energy [8].

The fission model implemented so far in McGNASH is identical to what is present in the GNASH code. Fission probabilities are calculated from the quantum-mechanical transmission coefficient through a simple double-humped fission barrier, using uncoupled oscillators for the representation of the barriers [9]. The barrier penetrabilities are computed using the Hill-Wheeler formula for inverted parabolas. An additional parameter is used to account for level density enhancement due to asymmetry at saddle points. This model is very simple and could be improved in several ways. One of them concerns the coupling of the two potential wells and the fluctuations arising because of this coupling, as described by Lynn in Ref. [11]. Another important improvement would be to use the microscopic-macroscopic fission model by Möller [12] to describe the different saddle points and the corresponding different paths to fission. Finally, a more realistic description of the fission path is not always very well fitted with parabolas [10]. Therefore, we plan to develop a new method to calculate fission transmission coefficients through an arbitrary barrier shape. These three new developments are planned for future releases of the code.

In GNASH, the pre-compound stage for neutron emission is calculated using the semi-classical exciton model as formulated by Kalbach in the code PRECO [13]. In this model, the excited nuclear system follows a series of ever more complicated configurations, where more

and more particle-hole states are excited. A version of GNASH also exists that implements the quantum-mechanical treatment of Feshbach-Kerman-Koonin [14]. In McGNASH, the DDHMS Monte Carlo code by Chadwick and Blann is used [15, 16]. While still semi-classical, the Hybrid Monte Carlo model has several and important advantages over the exciton model. In particular, it is not limited to low-order exciton densities, and can treat multiple emissions of precompound nucleons. Finally, the choice of a Monte Carlo algorithm really simplifies the treatment of exclusive reactions. In particular, the DDHMS code can be used to predict the residual spin distribution of the excited nucleus after the emission of preequilibrium nucleons. This distribution can differ significantly from the Hauser-Feshbach compound nucleus spin distribution, depending on the number and energy of the preequilibrium ejectiles. In applications particularly sensitive to the conservation of angular momentum (e.g., branching ratios to spin isomers, or precise determination of γ -ray lines in a gamma-cascade), it is important to calculate this residual spin distribution accurately. An example of such calculated residual spins distributions after preequilibrium emission is shown in Figure 2 for proton (160 MeV) on ^{90}Zr .

At low-incident energies, the statistical approximation that entrance and exit channels are independent (Bohr independence hypothesis) is not valid anymore due to interferences in the elastic channel. The Hauser-Feshbach equations have to be modified in order to include the so-called width fluctuation correction factors. Over the years, three models (Moldauer [17], HRTW [18] and exact GOE [19]) have been developed to estimate these correction factors [20]. We have implemented all three models directly in McGNASH. To do so, the usual Hauser-Feshbach loops have to be expanded to include the coupling between the incident and outgoing waves in the elastic channel. This difference in implementation is required only for the first compound nucleus decay. On the contrary, the GNASH code does not calculate these correction factors but rather import them as the result from an auxiliary code (usually, COMNUC). In addition to be cumbersome, this procedure does not lead to quite consistent results, although it has been proven to be a very good approximation in most physical situations. The result of a test calculation performed using McGNASH is shown in Figure 3.

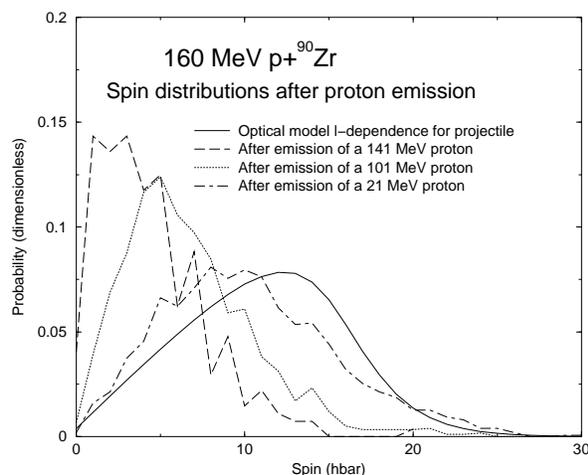


FIGURE 2. Proton-induced reaction on ^{90}Zr with $E_p=160$ MeV: residual spin distributions after the emission of a preequilibrium proton, as calculated with the DDHMS code, and compared to the compound nucleus spin distribution.

CONCLUSION

We have been working on a modern version of the GNASH statistical/preequilibrium nuclear reaction code. This new code, called McGNASH, is written in modern Fortran 95 scientific computing language. Although still

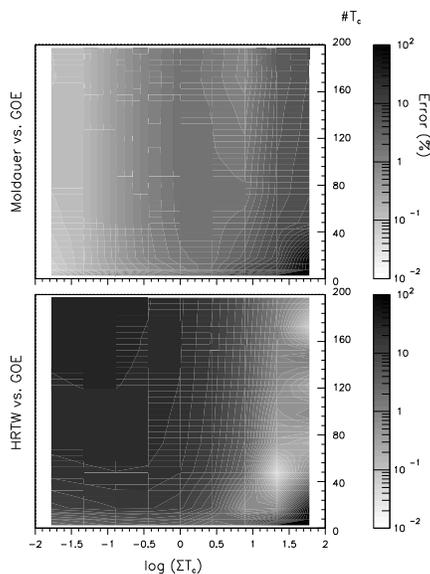


FIGURE 3. Comparison of HRTW, Moldauer and exact GOE approaches to the calculation of width fluctuation correction factors. The exact GOE approach is used as reference, and the errors due to the HRTW and Moldauer approximate formulas are computed as a function of the number of open channels or transmission coefficients ($\#T_c$) and their sum (ΣT_c).

in a preliminary version, the code already includes the most important physics models present in GNASH, and some extra features not present in GNASH (e.g., width fluctuation corrections and exclusive spectra). Its use is greatly simplified thanks to a very compact input file, complemented by default nuclear data files (e.g., from the RIPL-2 database) needed to run this type of nuclear reaction calculations. From the developer point of view, the code is being written with robustness and ability to evolve in mind, so that improvements can be developed quickly and efficiently without having to re-write most of the code. We plan the first release of McGNASH by the end of 2005. It will come as a package containing the source code, numerous test cases (input/output files), and a detailed manual.

ACKNOWLEDGMENTS

We acknowledge the help of Dr. S. Hilaire and Andres Morey for the implementation of the width fluctuation correction factors in McGNASH, and Dr. S. Lemaire for the development of the fission module.

REFERENCES

1. P.G. Young, E.D. Arthur and M.B. Chadwick, Proc. Workshop on *Nuclear Reaction Data and Nuclear Reactors*, ICTP, Trieste, Italy, April 15 - May 17, 1996 [World Sci. Publ. Co., Singapore (1998)] p. 227-404.
2. M.B. Chadwick *et al.*, Nucl. Sci. Eng. **131**, 293 (1999).
3. "Reference Input Parameter Library RIPL-2", <http://www-nds.iaea.org>.
4. J. Raynal, CEA Saclay Report No. CEA-N-2772 (1994).
5. O. Bersillon, *Progress Report of the Nuclear Physics Division, Bruyères-le-Châtel 1977*, CEA-N-2037, p. 111 (1978).
6. J. Kopecky and M. Uhl, Phys. Rev. **C41**, 194 (1990).
7. "DSD code", T. Kawano (private communication (2004)).
8. A.V. Ignatyuk, G.N. Smirenkin, and A.S. Tishin, Sov. J. Nucl. Phys. **21**, 255 (1975).
9. S. Bjornholm and E.J. Lynn, Rev. Mod. Phys. **52**, 725 (1980).
10. S. Goriely, private communication (2004).
11. J.E. Lynn and A.C. Hayes, Phys. Rev. **C67**, 014607 (2003).
12. P. Möller, D.G. Madland, A.J. Sierk, and A. Iwamoto, Nature **409**, 485 (15 Feb. 2001).
13. C. Kalbach, CEN Saclay Report Dph-N/BE/74/3 (1974).
14. H. Feshbach, A. Kerman, and A. Koonin, Ann. Phys. (N.Y.) **125**, 429 (1980).
15. M. Blann, Phys. Rev. **C54**, 1341 (1996).
16. M. Blann and M.B. Chadwick, Phys. Rev. **C57**, 233 (1998).
17. P.A. Moldauer, Nucl. Phys. **A344**, 185 (1980).
18. H.M. Hofmann, J. Richert, J.W. Tepel, and H.A. Weindenmüller, Ann. Phys. (N.Y.) **90**, 403 (1975).
19. J.J.M. Verbaarschot, Ann. Phys. (N.Y.) **168**, 368 (1986).
20. S. Hilaire, Ch. Lagrange, and A.J. Koning, Ann. Phys. (May 2003).