General ideas for coupling TALYS with GEF

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1. Introduction

This is a non-exhaustive list of possible coupling schemes for running TALYS together with the general fission model GEF. There is a fundamental difference in internal organisation: While TALYS calculates all decay probabilities and particle properties by folding in one passage, GEF is organised as a Monte-Carlo code where each reaction follows a specific decay path and the final distributions are built up by running the code many times.

Generally speaking, the folding method provides all reactions, also those with very low probabilities, within a relatively short computing time. This important advantage, however, is accompanied with a loss of correlations between the different observables. The characteristics of the Monte-Carlo method are just opposite: The computing time increases with the sensitivity of the calculation, but all correlations between the different observables are preserved. For many applications, some of these correlations are essential, and thus a pure folding version of the code assembly does not cover all needs, although it is a very efficient way for obtaining restricted information, e.g. on the nuclide production in fission.

2. Adapting GEF to the folding method

An homogeneous code assembly would require to produce a modified GEF version that uses the folding method. This is technically possible. Since the coupling of TALYS and GEF is direct, it is convenient to call a GEF subroutine in FORTRAN.

2.1. Basic solution

A consistent solution would be the coupling of TALYS with a a modified version of GEF that uses the folding method. In a basic version, TALYS calls a GEF subroutine with the list of fissioning nuclei and their respective excitation-energy and spin distribution. GEF returns arrays of primary fission fragments, with their respective excitation-energy and spin distribution. TALYS continues treating the de-excitation process, replacing the distributions of fissioning compound nuclei (composition in N and Z, probabilities and properties) by equivalent distributions of fission fragments (composition in N and Z, probabilities and properties). The number of nuclei to follow just doubles. This is the only modification needed in TALYS.

This solution is fast, but it looses all correlations between the complementary fission fragments, e.g. by the conservation of the total number of protons and neutrons or by the total kinetic energy. Nevertheless, this option produces fission-fragment yields (pre- and post-neutron), prompt-neutron and prompt-gamma spectra and yields of the individual fragments. However, kinetic energies of the fragments and total prompt-neutron yields cannot be obtained, because these require the knowledge of the correlations between the two complementary fragments.

Since the coupling of TALYS and GEF is direct, it is convenient to call a GEF subroutine in FORTRAN.

2.2 Following the de-excitation in GEF

Since there is a simple evaporation code included in the GEF code, this code may also be used to calculate the prompt-neutron and prompt-gamma emission from the fragments in the folding version of GEF. However, this evaporation code is structured as a Monte-Carlo code. Thus, one would have to call it many times in order to build up the corresponding distributions. This way, one would loose part of the good performance of a pure folding-type code.

2.3. Solution with partial correlations

It is in principle possible to preserve some of the correlations between the two complementary fragments in a folding version of the GEF code by increasing the number of dimensions. E.g. one may add the information of the fission channel or of the fissioning nucleus. This method is, however, limited by the increasing amount of memory required for the output of GEF. Furthermore, the construction of the complex output of arrays in GEF becomes complicated.

But there is a solution that avoids these problems. An additional dimension may also be realized by the calling sequence: If the GEF code is called by TALYS for each compound nucleus separately, the conservation of the number of protons and neutrons in the the two complementary fragments can be respected. If, in addition, the GEF code is called in a sequence of compound-nucleus excitation energies, it is possible to construct, at least with some approximate assumptions, total kinetic energies and total prompt-neutron and prompt-gamma yields.

3. Using the Monte-Carlo version of GEF

A mixed-method approach avoids the loss of information of the full folding-method approach described in chapter 2. The coupling of TALYS and GEF is less direct. It may be well adapted to couple the code by information exchange via a file. Thus, the problem of computer language is less severe. It could be advantageous to keep the FreeBASIC version of GEF, because this option simplifies the maintaining and further development of the code, since the original stand-alone version is written in FreeBASIC. The necessary modifications on the GEF code for this solution are minor. They can directly be included in the original stand-alone version.

3.1 List-mode output of GEF

If one does not want to loose the full information of correlations between the fission observables, one may couple TALYS with the Monte-Carlo version of GEF. The full information available in GEF is too large to be transported by multi-dimensional arrays. The most adapted way of transportation is a file with list-mode-structured events, where all properties and observables are listed for each fission event (see below). The desired information may then be extracted and analysed from these data. This is the simplest, the most versatile and most powerful solution for coupling TALYS with GEF.

<u>*Parameters provided in the list-mode output of GEF:*</u>

M: Fission mode
Z1: Atomic number of the first fission fragment
Z2: Atomic number of the second fission fragment
A1pre: Mass number of the first fission fragment before prompt-neutron emission
A2pre: Mass number of the second fission fragment before prompt-neutron emission
A1post: Mass number of the first fission product after prompt-neutron emission
A2post: Mass number of the second fission product after prompt-neutron emission
I1: Angular momentum of the first fission fragment before prompt-neutron emission
I2: Angular momentum of the second fission fragment before prompt-neutron emission
n1; Number of prompt neutrons emitted from the first fission fragment
n2: Number of prompt neutrons emitted from the first fission fragment
Eni: Energies of the prompt neutrons

TKEpre: Total kinetic energy before prompt-neutron emission
TKEpost: Total kinetic energy after prompt-neutron emission

In addition, the number and energies of the prompt gammas as well as several additional parameters may be provided.

A convenient and efficient coupling would be realized by calling GEF by TALYS in a sequence of fissioning nuclei, excitation energy and angular momentum.

3.2 Analysis provided by GEF

The present stand-alone Monte-Carlo version of GEF provides already an analysis of the complex information in terms of tables. This analysis part may be modified or extended according to specific needs. This solution avoids the output and the separate analysis of the list-mode data. However, the development of a separate analysis code (section 3.1) on the basis of the list-mode data is simpler and more transparent.

4. Conclusion

As a conclusion it might be appropriate to develop two coupling schemes. A pure folding solution is efficient and simple to use, since TALYS and GEF are directly coupled in an homogeneous code system in FORTRAN. This solution is best suited for cases where the restricted information provided by this version is sufficient. A mixed folding-Monte-Carlo solution is most versatile, because it preserves all kind of correlations. This version complies with more demanding needs of many applications. In this case, the stand-alone version of GEF can directly be used. The standard analysis part of the stand-alone GEF code may even cover the needs for many applications, avoiding the need for an additional analysis program.