Improved predictions of nuclear reaction rates for astrophysics applications with the TALYS reaction code

S. Goriely*
Institut d'Astronomie et d'Astrophysique, Université Libre de Bruxelles, Campus de la Plaine CP 226, B-1050 Brussels, Belgium

S. Hilaire
CEA, DAM, DIF, F-91297, Arpajon, France

A. J. Koning
Nuclear Research and Consultancy Group, P.O. Box 25, NL-1755 ZG Petten, The Netherlands
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Nuclear reaction rates for astrophysics applications are traditionally determined on the basis of Hauser-Feshbach reaction codes which make use of a number of approximations that have never been tested, such as a simplified width fluctuation correction, the neglect of delayed or multiple particle emission during the electromagnetic decay cascade, or the absence of the pre-equilibrium contribution at increasing incident energies.

Thanks to the developments brought to the TALYS reaction code, in particular to estimate Maxwellian-averaged reaction rates, we can now predict with an increased accuracy and reliability those of astrophysical relevance and test the aforementioned approximations. We show that TALYS predictions may significantly differ from those obtained with other codes, in particular for nuclei for which no or little nuclear data is available. Also, the pre-equilibrium process is shown to influence the astrophysics rates of exotic neutron-rich nuclei significantly. Finally, the Maxwellian-averaged (n,2n) reaction rate is calculated for all nuclei and its competition with the radiative capture rate discussed.

I. INTRODUCTION

Strong, weak, and electromagnetic interaction processes play an essential role in many different applications of nuclear physics, such as reactor physics, waste incineration, production of radioisotopes for therapy and diagnostics, charged-particle beam therapy, material analysis, and nuclear astrophysics. Although significant effort has been devoted in the past decades to measure reaction cross sections, experimental data only covers a minute fraction of the entire data set required for such nuclear physics applications. Reactions of interest often concern unstable or even exotic (neutron-rich, neutron-deficient, superheavy) species for which no experimental data exist. Given applications (in particular, nuclear astrophysics and accelerator-driven systems) involve a large number (thousands) of unstable nuclei for which many different properties have to be determined. Finally, the energy range for which experimental data is available is restricted to the small range that can be studied by present experimental setups. To fill the gaps, only theoretical predictions can be used.

In astrophysical applications, reaction rates for medium or heavy nuclei have been calculated until now on the basis of the Hauser-Feshbach (HF) statistical model [1], adopting simplified schemes to estimate the capture reaction cross section of a given target nucleus, not only in its ground state but also in the different thermally populated states of the stellar plasma at a given temperature [2–9]. Such schemes include a number of approximations that have never been tested, such as the neglect of delayed particle emission during the electromagnetic decay cascade or the absence of the pre-equilibrium contribution at increasing incident energies or for exotic neutron-rich nuclei.

In parallel, the nuclear physics community has developed tools for specific applications, such as accelerator-driven systems, which can shed light on the many approximations in nuclear astrophysical applications. One of these tools is the TALYS nuclear reaction code [10] which includes many state-of-the-art nuclear models to cover all main reaction mechanisms encountered in light particle-induced nuclear reactions. It provides a complete description of all reaction channels and observables and in particular takes into account all types of direct, pre-equilibrium, and compound mechanisms to estimate the total reaction probability as well as the competition between the various open channels. The code is optimized for incident projectile energies, ranging from 1 keV up to 200 MeV on target nuclei with mass numbers between 12 and 339. It includes photon, neutron, proton, deuteron, triton, 3He, and α-particles as both projectiles and ejectiles, and single-particle as well as multi-particle emissions and fission. All experimental information on nuclear masses, deformation, and low-lying states spectra is considered, whenever available [11] and if not, various local and global input models have been incorporated to represent the nuclear structure properties, optical poten-

*Electronic address: sgoriely@astro.ulb.ac.be

tials, level densities, γ-ray strengths, and fission properties. The TALYS code was designed to calculate total and partial cross sections, residual and isomer production cross sections, discrete and continuum γ-ray production cross sections, energy spectra, angular distributions, double-differential spectra, as well as recoil cross sections. We have updated TALYS to estimate reaction rates of particular relevance to astrophysics. In contrast to other codes developed for astrophysical applications, TALYS avoids many of the approximations mentioned above and therefore provides a unique opportunity to test them.

II. IMPACT OF SOME OF THE TALYS ADDED VALUES

Concerning the calculation of Maxwellian-averaged reaction rates of astrophysical interest, the TALYS code has some clear advantages over previous codes developed for astrophysical applications (like MOST), such as :

– the inclusion of the pre-equilibrium reaction mechanism (totally neglected in other astrophysical nuclear codes);

– the detailed description of the decay scheme, including the description of γ-delayed particle emission and the possible particle emission from all residual nuclei. In astrophysical codes, the particle emission following a primary γ cascade is not explicitly taken into account, but corrected roughly by artificially reducing the photon transmission coefficient in as described by Holmes et al. [3];

– the inclusion of multi-particle emission (totally neglected in other astrophysical nuclear codes);

– the inclusion of detailed width fluctuation corrections [12] in contrast to the approximation of Hofmann et al. [13, 14] applied in other astrophysical codes;

– the inclusion of parity-dependent level densities (the parity equipartition is usually assumed in astrophysical codes, one exception being the work of Mocelj et al. [15], which however considers a spin-independent parity distribution);

– the inclusion of a coupled channel description for deformed nuclei, while the other astrophysical codes consider spherically equivalent optical potentials for deformed targets;

– the inclusion of the fission channel for the compound as well as the residual nuclei. Fission is often neglected in astrophysical codes, and if included, insufficiently tested on experimental data and not consistently taken into account in the full decay scheme.

For the calculation of thermonuclear reaction rates at astrophysical relevant temperatures, most approximations assumed by previous codes are justified since, for neutron captures, only incident energies of a few keV to 1 MeV contribute, and, for incident charged particles, only energies below or close to the Coulomb barrier come into play. Therefore, the above mentioned added values do not usually affect the predicted rates by more than a few tens of a percent and remain insignificant with respect to the uncertainties in the nuclear ingredients, such as nuclear properties, level densities, or γ-ray strengths. However, in some specific astrophysical applications, highly accurate predictions may be required.

A first example is the the Re-Os nucleocosmochronology, which is known to be sensitive to the estimate of the ^{187}Os(n,γ)^{188}Os reaction rate and most particularly to the experimentally unknown contribution of the thermally populated 9.75 keV first excited state of ^{187}Os. A significant amount of experimental data has been gathered to constrain the determination of this reaction rate directly or indirectly [16]. In this specific example, to reconcile all of the direct and indirect constraints obtained experimentally, the state-of-the-art reaction model should be used, and in particular a proper description of the width fluctuations is required. As already mentioned, the TALYS code enables the neutron capture rates to be estimated with different prescriptions for the width fluctuation correction. In particular, the exact, but very computer-time-consuming, Gaussian Overlap Ensemble (GOE) approach of Verbaarschot et al. [17] or its excellent approximation due to Moldauer [18] can be used as well as the correction of Hofmann et al. [13, 14], traditionally adopted in all previous works related to the Re-Os chronology. As can be seen in Fig. 1, this latter prescription differs by some 40% from the GOE predictions at the relevant low temperatures (below some 3×10^8 K), and, as detailed in Ref. [16], such a difference significantly affects the determination of the stellar ^{187}Os(n,γ)^{188}Os reaction rate, and, consequently, the determination of the age of the Galaxy.

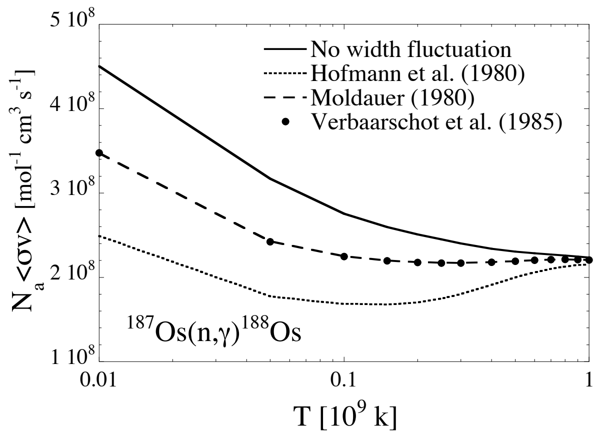

FIG. 1: Stellar ^{187}Os(n,γ)^{188}Os rate as a function of the temperature for 3 different prescription of the width fluctuation correction and without any.

Another illustrative example is the impact of the pre-equilibrium process. Pre-equilibrium emission occurs after the first stage of the reaction but long before statistical equilibrium of the CN is achieved, leading to the well known high-energy tails in the emission spectra and the smooth forward peaked angular distributions. This process is also responsible for the observed increase in the radiative neutron-capture cross section for stable nuclei at incident energies typically around 10 MeV (see e.g. upper panel of Fig. 2). If this can hardly affects the Maxwellian-averaged reaction rates of astrophysical relevance, this is not the case for exotic neutron-rich nuclei with low neutron separation energies. Indeed, for such nuclei, the low-level density makes it difficult for the nucleus to achieve complete equilibrium, and the pre-equilibrium process starts to affect the neutron channel already at a few hundred keV, and consequently may change the astrophysical rate. This is illustrated in Fig. 2, where it can be seen that already at 100 keV, the pre-equilibrium

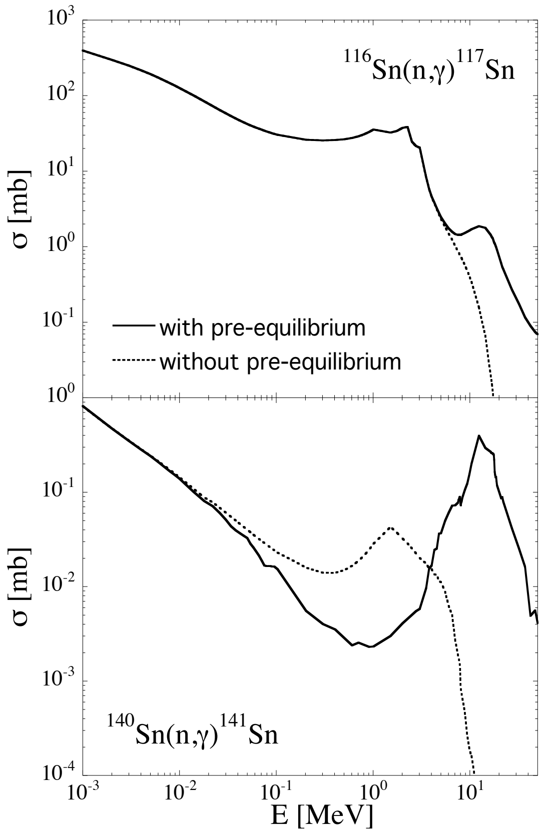

FIG. 2: Radiative neutron capture cross section for ^{116}Sn (top) and ^{140}Sn (bottom) with and without including the pre-equilibrium processes as a function of energy.

process modifies the capture cross section of ^{140}Sn, while for ^{116}Sn, it only contributes above some 7 MeV. We note that the pre-equilibrium model adopted here corresponds to the two-component exciton model [19], which remains relatively phenomenological. Its reliability and quantitative contribution, when applied to neutron-rich nuclei, can therefore be questioned. However, such an effect is found to be qualitatively non-negligible for exotic neutron-rich nuclei of small neutron separation energies, regardless of the nuclear input adopted. The decrease in the reaction cross section for the 100 keV region affects directly the Maxwellian-averaged reaction rates of relevance to astrophysics as seen in Fig. 3 (upper panel). At increasing temperatures, the Gamow energy increases and overlaps the energy region in which the pre-equilibrium process contributes to the reaction mechanisms. The pre-equilibrium correction is found to be less important for odd-N target nuclei than for even-

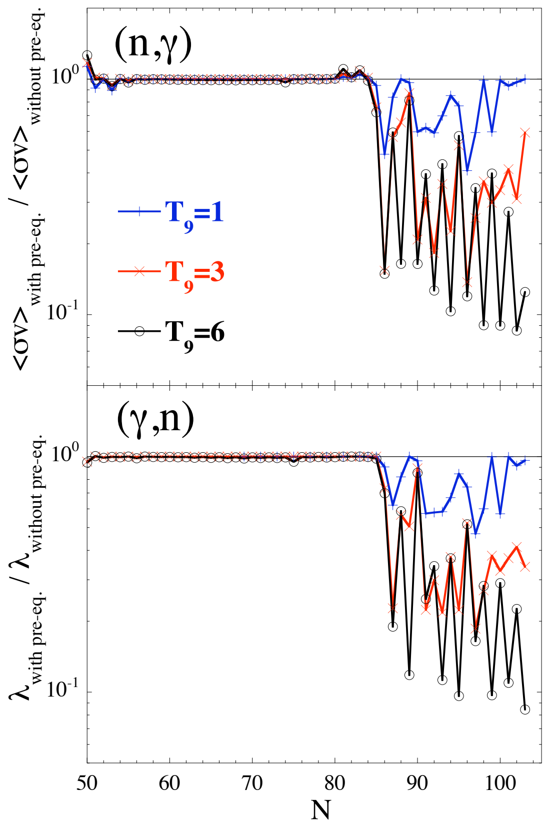

FIG. 3: Ratio of the radiative neutron capture (top) and photoneutron (bottom) rates obtained with and without inclusion of the pre-equilibrium contribution for all Sn isotopes at 3 different temperatures.

N. This is essentially due to the increase in the HF cross section for the 0.52 MeV region found for even-N target nuclei, which results from the oddness of the compound system that has a larger nuclear level density and the evenness of the target reducing the inelastic channel competition. The pre-equilibrium contribution is found to decrease not only the radiative capture, but also the (n,2n) reaction rates of neutron-rich nuclei at temperatures around $T \approx 2-4\times 10^9$ K by about 50%. It affects not only the nucleon or α-particle capture rates but also the photoneutron rates of neutron-rich nuclei, as illustrated in Fig. 3 (lower panel). Since the pre-equilibrium component contributes increasingly more as energies increase, the higher the temperature the larger the impact on the astrophysics rates, as seen in Fig. 3. The impact is also observed to be stronger for odd-N compound nuclei (i.e. for the neutron capture by an even-N target or the photoneutron emission of an odd-N target).

Last but not least is the possibility that the TALYS code offers to deal with multi-particle emission. Indeed, All reaction codes dedicated to astrophysical applications have made the simplified assumption that the contribution of the emission of more than one particle in neutron or charged-particle induced reactions is negligible. In most astrophysical scenarios, the temperatures are indeed sufficiently low for such channels not to compete. However, it remained impossible to test such an approximation, because until now, no reaction code for astrophysical applications has included the multi-particle emission in their framework. By applying the TALYS code, it is possible to have a more robust understanding of the competing channels that until now have been neglected. An important one is the (n,2n) channel that may dominate, at relatively high temperatures, the (n,γ) channel, especially for exotic neutron-rich nuclei. For energies above the two-neutron separation energies, the (n,2n) channel is open and begins to dominate very quickly, so that at a given temperature the ratio $r_n =< \sigma v >_{\rm (n,2n)} \; / \; < \sigma v >_{\rm (n,\gamma)}$ becomes larger than 1. This temperature is critical in applications such as the r-process nucleosynthesis, since above such a temperature, the neutron capture will not lead to the production of heavier neutron-rich nuclei, but in contrast will start to

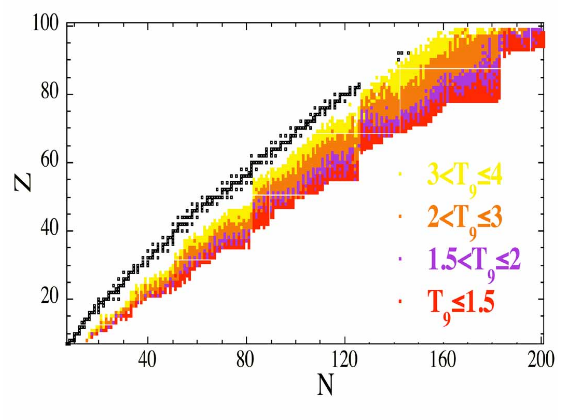

FIG. 4: Representation in the (N,Z) plane of the critical temperature T_9 (see text) at which the Maxwellian-averaged (n,2n) rate becomes faster than the (n,γ) rate (i.e. $r_n = 1$).

reverse the nuclear flow and prevent it from reaching the neutron-rich region. In Fig. 4, we show the evolution of the critical temperature in the (N, Z)-plane. It can be seen that at temperatures above 3×10^9K ($T_9 \geq 3$), most of the neutron-rich region cannot be reached by neutron captures regardless of the neutron density in the astrophysical environment. At T9 = 3 for example, within the Cd or Sn isotopic chain, the r-process flow could not reach isotopes heavier than ^{131}Cd or ^{133}Sn, respectively. At such high temperatures, the (n,2n) channel represents a nuclear barrier that the r-process flow would not be able to cross, independently of the amplitude of the neutron density. The nuclear flow into the neutron-rich region is usually believed to be stopped by photodissociation. However, this (γ,n) barrier at a given temperature can always be counterbalanced by considering higher neutron densities, while the (n,2n) competition represents a barrier to the (n,γ) flow independent of the neutron density. This nuclear barrier could significantly modify the prediction of the resulting r-abundance distribution, should the r-process develop in such a high-temperature environment. The temperature at which the r-process occurs remains however unknown.

III. REACTION RATES SENSITIVITY

We have seen that the added values of TALYS can have significant impacts on the predictions of the reaction rates of astrophysical relevance, and that these impacts are generally more important for exotic nuclei than for nuclei close to stability. These conclusions are also true when TALYS predictions are compared with those of the

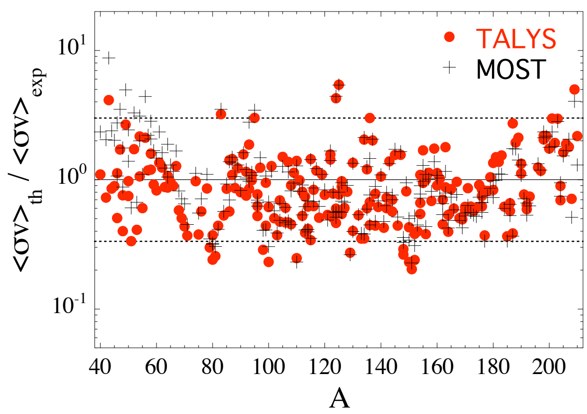

FIG. 5: Comparison of the Maxwellian-averaged (n,γ) rates at $T = 3 \times 10^8$K obtained using either the TALYS (red circles) or the MOST (crosses) code with the experimental Maxwellian-averaged data compiled by Bao [30] above Ca.

widely used [9, 20] MOST code as done in Fig. 5. The two codes have been employed with almost the same nuclear inputs. They both reproduce the experimental data with the same accuracy (i.e. within roughly a factor of 2-3. Little differences can however be noticed. They are partly due to the fact that few differences exist between the MOST and TALYS databases of experimental structure properties, in particular in the way deformation effects are considered. In MOST, for instance, the Fe-group nuclei are described as rotationally deformed while the same nuclei are rather considered as vibrators in TALYS. If we extend the comparison to more exotic neutron rich nuclei involved in the r-process (see Figs. 3 and 4 of Ref. [21]) deviations by a factor as large as 10 can be obtained as soon as nuclei away from the valley of stability are considered.

It is also possible with TALYS to study the impact not only of the nuclear model parameters but also of the nuclear models themselves. Indeed, as indicated in Table I, most of the macroscopic model included in TALYS can be replaced by an alternate microscopic counterpart. Microscopic models are believed to be of higher reliability due to their sound physical bases and therefore better suited for extrapolation far away from experimentally known regions of the nuclear chart. Such models have been shown to predict experimental data with the same degree of accuracy as the more phenomenological models traditionally used for practical applications. The predictions obtained using either the microscopic ingredients or the macroscopic ones are compared with experimental data in Fig. 6. One can clearly see that the microscopic ingredients reproduce experimental (n,γ) rates with an accuracy similar to that obtained using the more traditional macroscopic ingredients. For heavy isotopes, the agreement with experiment is even better when microscopic ingredients are used. This confirms that the microscopic ingredients are as good as the macroscopic ones for nuclei close to the valley of β-stability as far as the astrophysical rates are concerned. When looking at exotic nuclei for which there are not any experimental data, one can only compare the astrophysical relevant rates obtained using microscopic ingredients with those obtained thanks to the macroscopic ones. This comparison is performed in Fig. 7 and shows very different predictions are obtained for nuclei far away from the valley of stability.

TABLE I: Macroscopic and microscopic model ingredients implemented in TALYS.

NUCLEAR INGREDIENTS	"MACROSCOPIC"	"MICROSCOPIC"
Ground State Properties	FRDM [22]	HFB-13 [23]
Nuclear Level Densities	BSFG [24]	HFB Combinatorial [25]
E1-γ Strength functions	Lorentzian [26]	HFBCS+QRPA [27]
Optical Potentials	Woods Saxon [28]	JLMB soon [29]

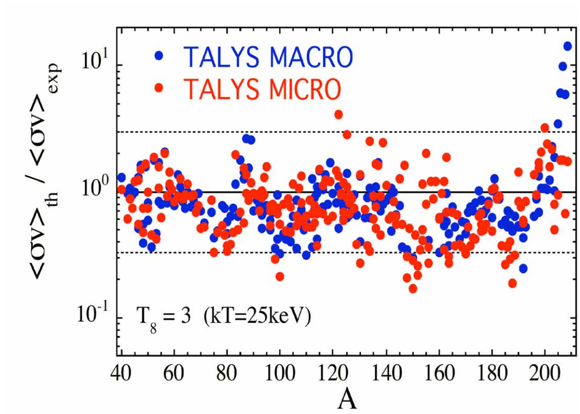

FIG. 6: Comparison of the Maxwellian-averaged (n,γ) rates at $T = 3\times10^8$K obtained using either microscopic (red circles) or macroscopic (blue circles) nuclear ingredients (see Table I) with the experimental Maxwellian-averaged data compiled by Bao [30] above Ca.

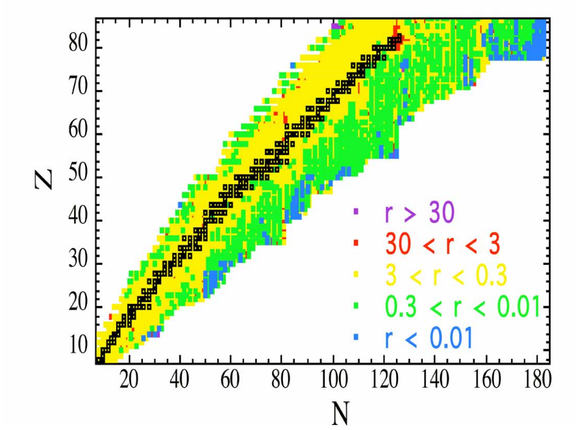

FIG. 7: Representation in the (N,Z) plane of the ratio of the radiative neutron capture rates obtained using macroscopic nuclear ingredients with the rates obtained using microscopic ingredients for a temperature of 10^9K ($T_9 = 1$).

IV. CONCLUSIONS

The reaction code TALYS has undergone several developments, in particular to estimate the Maxwellian-averaged reaction rates of particular relevance to astrophysics using microscopic nuclear models for ground state properties, nuclear level densities, γ-ray strength functions, and nucleon-nucleus optical potentials. These developments enable the reaction rates to be estimated with improved accuracy and reliability, and the approximations, assumed until now by other codes, to be tested. The TALYS predictions for the thermonuclear rates are found to be relatively similar to the more traditional astrophysics codes for stable nuclei, but major differences are obtained when considering exotic neutron-rich nuclei. In particular, the pre-equilibrium process, neglected in previous astrophysical-orientated reaction codes, is found to play an important role at low energies, at least for neutron-rich nuclei. TALYS can also estimate the multi-particle emission cross sections in photon and particle-induced reactions that have been until now neglected. Within this context, the (n, 2n) channel is found to become important at increasing temperatures and even to dominate, at relatively high temperatures, the (n,γ) channel, for exotic neutron-rich nuclei. The presence of such a (n, 2n) barrier demonstrates that the neutron captures characterizing the r-process nucleosynthesis could not occur at temperatures above typically $T = 3 \times 10^9$ K. TALYS presents additional advantages such as the detailed description of the decay scheme, the inclusion of accurate width fluctuation corrections, the inclusion of parity-dependent level densities or a proper description of the deformation effects. The impact of such features on reaction rates of relevance to astrophysics and on astrophysical observables remains to be further studied in the future.

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