Systematic and correlated nuclear uncertainties in the i-process at the neutron shell closure $N = 82$

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Nuclear astrophysics simulations aiming to study the origin of the elements in stars require a multitude of nuclear physics input. Both systematic model dependent and statistically correlated uncertainties need to be considered. An application where realistic uncertainty assessments are especially important is the intermediate neutron capture process or i process: a neutron capture regime with neutron densities intermediate between the slow and rapid processes. Accordingly, the main network flux proceeds on the neutron-rich unstable isotopes up to 4-5 species off the valley of stability. The i process has been clearly identified to be active in post-AGB stars during the Very Late Thermal Pulse II-ingestion event, and a recent work infers about its important role in early generations of stars. Here we demonstrate the effect of propagating systematic nuclear uncertainties from different theoretical models to final abundances for a region around the 2nd peak at $A - Z = 80$ for elemental ratio predictions involving Ba, La and Eu in i-process conditions. These elements are used to distinguish different n-capture contributions observed in low-metallicity stars. For the simple 1-zone model adopted here, predictions vary as much as a factor of 22 in on possible observational plane ($[\text{La}/\text{Eu}]$ vs. $[\text{Ba}/\text{La}]$). To consider statistically correlated uncertainties, we similarly perform a full nuclear physics uncertainty study within a given Hauser-Feshbach model and demonstrate the role of correlations on the final stellar abundance uncertainties. We show that in i-process conditions the main result of neglecting correlations is to underestimate the impact of nuclear uncertainties on the final nucleosynthesis yields by as much as two orders of magnitude. In the mass region of the neutron shell closure $N = 82$ Cs final abundances are most affected by correlated nuclear uncertainties with an uncertainty of about a factor of 3.5 compared to a factor of $6 \times 10^{-3}$ when uncorrelated nuclear uncertainties are used. In both cases Te and I final abundances show a negligible effect.

I. INTRODUCTION

Nuclear physics for stellar nucleosynthesis simulations include charged and uncharged nucleon-nucleus and nucleus-nucleus cross sections as well as weak rates. Already Caughlan and Fowler [1] (see also references therein) emphasized the importance of nuclear reaction rates as a crucial aspect of stellar modeling. Now, several stellar reaction rate libraries exist such as JINA REACLIB [2], NACRE [3], and KaDoNIS [4]. Rates within these libraries are based on experiment, where available, and theory elsewhere, and usually include some information of the uncertainty of the individual rates.

As the fidelity of stellar astrophysics simulations and astronomical observations of stellar abundances has been continuously increasing, new nuclear astrophysics applications in astronomy have emerged. These include, for example, near-field cosmology [e.g. 5, 6], the discovery and interpretation of the most metal-poor stars in the galaxy [7, 8] and the investigation of the formation and evolution of the first structure and stars in the universe [e.g. 9–11].

Stars of very low metallicity probe the conditions for nuclear production in the early universe. They often show highly non-solar abundance distributions, such as the C-enhancements in a large fraction of metal poor stars (the C-enhanced metal poor or CEMP stars) that are often correlated with strong enhancements of transition elements [7]. Both r-process (such as Eu) and s-process element (such as La and Ba) enhancements are found. Indeed, a number of CEMP stars show an s-process signature close to what s-process simulations predict. For example the CEMP-s stars HD196944 [12] has $[\text{La}/\text{Eu}] = 0.74$ while s-process models for the same Fe abundance predict a range of $[\text{La}/\text{Eu}] = 0.9 \ldots 1.0$ (see Roederer et al. [13], Table 3). Extensive comparisons are available in Bisterzo et al. [14] and Lugaro et al. [15]. The bona fide r-process stars are characterized by large Eu abundance and accordingly $[\text{La}/\text{Eu}] = -0.55$ [16]. Both stars are shown in a triple-element plot in Fig. 1 which separates the s- and r-process stars. However, it is clear that most stars lie between the s- and r-process extrema at $0.0 < [\text{La}/\text{Eu}] < 0.5$. These stars are usually referred to as the CEMP-r/s stars, indicating that somehow they carry the signature of both the s and r process.

Many scenarios have been suggested for the origin of the CEMP-r/s stars. Bisterzo et al. [14] construct models for a large number of CEMP-s and CEMP-r/s under
the assumption that CEMP-r/s stars get the r-process contribution from a pre-enriched cloud out of which a binary forms. The more massive companion will then first evolve to become an AGB star and pollute the secondary with the s-process elements. CEMP-s stars would form in the same way, except not out of an enriched cloud. The interpretation of their observational data lead Allen et al. \cite{17} to the conclusion that Eu must be produced along with Ba and C in low-metallicity AGB stars, the primaries of both CEMP-s and CEMP-r/s stars. However, as we pointed out above, this is in stark contrast to present models of n-capture nucleosynthesis in AGB stars, which insist that, e.g. the [La/Eu] ratio must be around one according to s-process models.

The possible importance of an intermediate neutron-density regime in very metal poor stars was proposed by Herwig et al. \cite{19}. Lugaro et al. \cite{20} discuss the possibility that an intermediate process in low-mass AGB stars, triggered by H ingestion, could be responsible for the signature in CEMP-r/s stars. However, this scenario would not explain the systematic larger enrichment of heavy element in CEMP-r/s stars compared to CEMP-s stars, and the preferential correlation with both carbon and nitrogen instead of with only carbon abundance \cite[e.g.,][]{21}. In this context Herwig et al. \cite{22} have proposed, based on new stellar evolution models, that a neutron-capture regime with neutron densities intermediate to the slow and rapid process, i.e. the i process with \( N_n \approx 10^{15} \text{cm}^{-3} \) \cite{23}, could be activated in super-AGB stars with Fe metallicities of \( [\text{Fe}/\text{H}] < -1.3 \). These super-AGB stars may be an efficient source of n-capture element enhanced ejecta with i-process signature, which in fact predicts [La/Eu] ratios in the range observed in CEMP-r/s stars. A related scenario with detailed nucleosynthesis simulations has been explored previously, for example, by Campbell et al. \cite{24} for the He-core flash, by Cristallo et al. \cite{25} for the first convective thermal pulse in low mass AGB stars at low metallicity and by Herwig et al. \cite{14} for the post-AGB star Sakurai’s object. Predictions of the latter work can be compared with detailed abundance observations which provide a unique validation opportunity. In addition, the i-process nucleosynthesis predictions for post-AGB stars have been recently shown to correspond to previously unexplained isotopic signatures measured in pre-solar grains \cite{26, 27}.

Generally speaking, at the high neutron densities of the i process the network flux proceeds parallel to the valley of stability, offset by approximately \( 1 - 6 \) mass numbers. Here, the role of accurate nuclear physics input becomes a critical issue. Where the experimental determination of precise cross sections for astrophysically relevant energies is difficult or impossible, large uncertainties may be introduced by theoretical reaction rates, where various models may produce orders of magnitude differences. For some time, the detailed evaluation of nuclear data from both theory and experiment has led to significant developments in the evaluated nuclear data libraries such as JENDL-4 \cite{28}, JEFF-3.1 \cite{29} and ENDF/B-VII.1 \cite{30}. Evaluated libraries are produced comprehensively through critical comparison, selection renormalization and averaging of the available experimental data with a region and are complemented by nuclear model calculations for specific nuclei within a region where experimental information may be unavailable.

In such libraries full uncertainty studies of each reaction may be included, obtained utilizing various statistical methods. However, the evaluated data libraries are often concerned with energy and isotopic regions not crucial to the astrophysical processes. Application of these rigorous uncertainty evaluation methods is of interest to the astrophysics community and has resulted in various sensitivity investigations of the stellar abundances as a function of nuclear reaction rate.

In particular, the past decade has produced several studies on the role of neutron capture rates in nucleosynthesis processes, and their effects on individual isotopes \cite{31, 32}. Sensitivity studies of this sort, considering only the effects of changes to single reaction rates, are critical for informing which reaction rates are dominant in a given stellar environment. They are a first step in providing a complete uncertainty study of the the nuclear physics input. However, there is no consideration of the systematic uncertainties among models or the uncertainty correlations inherent within a model. These considerations necessitate the inclusion of multiple neutron capture rates in the uncertainty study. Such an investigation is needed to determine if single reaction rate uncertainty studies provide sufficient insights to nucleosynthesis uncertainties beyond sensitivities.

In this paper we will demonstrate the propagation of systematic uncertainties among different theoretical
models for multiple neutron capture rates in a region of multiple importance to the interpretation of CEMP-r/s stars. This is the region around the i-process bottleneck $^{135}$I which determines the nucleosynthesis model prediction in the La-Eu-Ba plot (e.g. Fig. 11) that is particularly suited to distinguish between CEMP-s and CEMP-r/s stars.

This study begins with a description of the role of systematic uncertainties from varying reaction models. Additionally, we look at the effects of correlations in determining the full astrophysics uncertainty arising from a single neutron capture model. We will focus on the effects of theoretical neutron capture rate uncertainties from a Hauser-Feshbach statistical model including model correlations. The uncertainties within a given Hauser-Feshbach model are developed from physical motivation and propagated using a Monte Carlo method.

We investigate the role of large systematic uncertainties and the smaller statistically correlated uncertainties in overall neutron capture rate uncertainties in the i-process for 22 nuclei in the region around the neutron shell closure $N = 82$, where $N$ is the total number of neutrons in the nucleus. The results of propagating uncertainties indicate correlations are of significant importance to final abundance uncertainties and astrophysical conclusions. In Sec. III we will discuss how the neutron capture rates are calculated for a stellar environment and the applicability of the Hauser-Feshbach statistical method. Section IV looks at the proper treatment of uncertainties arising from neutron captures calculated using different Hauser-Feshbach models. In Sec. V we then consider a Monte Carlo approach to determine the neutron capture uncertainties within a single Hauser-Feshbach model and their propagation through the nucleosynthesis simulation. Finally, in Sec. VI we draw conclusions on the importance of correlations within astrophysical uncertainty studies.

II. NUCLEOSYNTHESIS IN THE I PROCESS

In order to analyze the impact of nuclear uncertainties on i-process calculations we use an ad-hoc 1-zone trajectory by Herwig et al. [22]. The 1-zone i-process trajectory is a simplified way of investigating nucleosynthesis at conditions typical for the H-$^{12}$C combustion in stellar evolution, such as the very-late thermal pulse (VLTP) in post-AGB star Sakurai’s object [38-40]. In the real star these events are characterized by the highly non-linear and non-spherically symmetric interaction of convective flows with violent nuclear burning that demand a full 3D-hydrodynamic treatment. However, spherically-symmetric multi-zone models can capture important elements of the nucleosynthesis that is encountered in these H-combustion events. The key defining property of i-process conditions is the very high neutron density of $N_n \sim 10^{12-14}$ cm$^{-3}$, which can be found in the He-shell flash convection zone of low-mass AGB stars where neutrons originate from the $^{23}$Ne-source. But it is also much lower than both n- and r-process conditions with $N_n \sim 10^{18}$ cm$^{-3}$ and $N_n > 10^{20}$ cm$^{-3}$ ([42] and [43], respectively).

In real stars i-process conditions can only be obtained in a 2-stage burning and mixing process. First, protons are convectively mixed down into a convectively unstable He-shell flash convection zone. The mixing time scale is of the order of $\sim 15$ minutes, and the temperature at which the $^{12}$C+p reaction time scale is approximately $1.1 - 1.5 \times 10^8$ K. At this point $^{13}$N forms, which is unstable with a half-life of 9.6 minutes. Because it has a higher Coulomb barrier than $^{14}$C its charged particle reaction cross sections are smaller, and it can be advected by convection to the bottom of the He-shell flash convection zone. Upon arrival and decay the resulting $^{13}$C will find itself at $T \sim 2.8 \times 10^8$ K and the neutron release happens almost instantly. If ample $^{13}$N is produced in the H-burning step then the neutron density is defined by the decay rate of $^{13}$N, which is model independent. This is the reason we expect nucleosynthesis conditions of a similar type, characterized by a typical neutron density, in a wider range of specific objects. This universality justifies identifying these conditions as a separate process, the i-process.

In the past we have studied the i-process conditions in multi-zone nucleosynthesis simulations [39]. However, in order to understand basic nuclear network path behaviors a 1-zone trajectory may be more adequate. We can create i-process conditions in a 1-zone trajectory in a relatively easy way assuming constant T and mass density $\rho$. We need to assume an initially high abundance of protons as well as $^{12}$C to create copious amounts of $^{13}$N. We use a temperature that is as high as possible without letting the $^{13}$N react with protons to form $^{14}$O, which would bypass the $^{13}$C neutron source. At the same time we need the temperature high enough to release neutrons from the $^{13}$C+p reaction as soon as possible after the decay of $^{13}$N. A 1-zone burning with constant temperature of $T = 2 \times 10^8$K and $\rho = 10^9$ g/cm$^3$, and an initial abundance of $X(^4\text{He})=0.2$, $X(^{12}\text{C})=0.5$ and $X(^{16}\text{O})=0.3485$ while all other species are according to the solar abundance distribution [44] accomplishes these constraints and provides a neutron density around $N_n \sim 10^{15}$ cm$^{-3}$ that is the defining criterion for the i-process.

The i-process 1-zone trajectory allows us to investigate general features of nucleosynthesis at such neutron density conditions. Just as the s process and the r process show characteristic properties due to the different number of unstable species involved in both processes, we can expect similarly specific signatures of i-process conditions, which are the result of a network flux departing much more significantly to shorter half lives away from the valley of stability than the s process, but not reaching the extremely unstable species like the r process.

It is well known that observed signatures of neither r
process nor s process can be explained by a single exposure \[45, 46\]. The same would have to be true for the i process. In the same way as the nucleosynthesis calculation along a single trajectory of a \(^{13}\)C pocket evolution extracted from a complete AGB stellar evolution model will give some idea of the general type of nucleosynthesis we can not hope to obtain accurate predictions of the details of a particular observation.

We expect the i-process 1-zone trajectory to provide some general idea of the type of nucleosynthesis that can be expected for environments in which we expect the i process to operate, for example in the H–\(^{12}\)C combustion regime in VLTP post-AGB stars, such as Sakurai’s object, or the various occasions of this type of events that are encountered in the low-Z stars that formed in the early universe.

The key ingredient of the i process is a combination of rapid proton capture (p-capture) nucleosynthesis with rapid neutron capture (n-capture) nucleosynthesis. In any realistic environment this combination is achieved by a convective connection of these two spatially separated regimes. The i-process 1-zone trajectory combines these two regimes in a serial fashion. In the first second all the \(^{12}\)C is burned into \(^{13}\)N. Several other p-capture induced reactions take place and overall the network flux drives species into the proton-rich side. Around 13.15 minutes, \(^{13}\)N decay starts to provide \(^{13}\)C and an increasing effect of the n-captures can be seen, as the flux is first drawing the abundance distribution back to the valley of stability and then driving the network flux into the neutron-rich side.

Neutrons are captured both by light elements as well as by iron and heavier elements. In particular, the neutron capture on the iron seeds leads quickly to the production of trans-iron elements Kr, Rb, Sr, Y, Zr around the first neutron-magic peak at \(N = 50\). It peaks initially and then decreases as the network flux moves on to the 2\(^{nd}\) peak around Ba and La at \(N = 82\). These elements peak somewhat later. The abundance distribution of Sakurai’s object is characterized by a large enhancement of 1\(^{st}\)-peak elements but no enhancement of 2\(^{nd}\) peak elements. Figure 2 shows the abundance flow at the two peaks for select times during the i process.

### III. NEUTRON CAPTURE RATES

Two primary nuclear physics inputs needed to determine the nucleosynthetic outcome are the neutron capture cross sections and rates. The neutron capture cross section \(\sigma_n\) may be determined several ways. Evaluated data on fission product \((n, \gamma)\) reactions is available in the various libraries \[28, 30\]. Additionally, one may calculate the capture cross section directly via the Hauser-Feshbach method \[47, 48\]. Hauser-Feshbach is a statistical method giving the cross section of reactions that pass through a large number of compound nucleus states \[47, 50\], and is implemented in available codes such as CoH\(3\) \[51\], TALYS 1.4 \[52, 53\] and NON-SMOKE\(R\) \[54\].

The reaction rate for neutron capture at a given stellar temperature \(T\) is given by the averaged product of the cross section \(\sigma_n\) and the relative velocity \(v\) between the neutron and target, obeying Maxwell-Boltzmann statistics. The Maxwellian averaged cross section (MACS) \((\sigma_n v)\) is then \[55\]:

\[
\langle \sigma_n v \rangle = \int_{\frac{\nu_m}{2}}^{\infty} \sigma_n v f(v) dv
\]

where \(f(v)\) is the Maxwell-Boltzmann distribution function with velocity \(v\), and \(\nu_m\) is the maximum velocity where \(f(v)\) goes to zero.
\[ \sigma_{\text{Maxw}} = \frac{\langle \sigma_\gamma v \rangle}{v_T} = \frac{2}{\sqrt{2\pi(kT)^2}} \int_0^\infty dE \sigma_\gamma(E)E \exp(-\frac{E}{kT}) \] (1)

where \( v_T = \sqrt{\frac{2kT}{\mu}} \) is the thermal velocity, \( E \) is the incident energy of the neutron, \( \mu \) is the reduced mass of the system and \( k \) is Boltzmann’s constant. The cross section \( \sigma_\gamma \) is the critical input and source of greatest uncertainty in determining the MACS. Section V details how we develop the full uncertainties in nucleosynthetic abundances from underlying uncertainties in a particular Hauser-Feshbach model.

### A. Applicability of Hauser-Feshbach

The Maxwellian temperatures in our astrophysical environment are typically in the keV regions, where the statistical Hauser-Feshbach calculations are appropriate. However, the statistical model does not give the \( 1/v \) cross section at very low energies, since it deals with energy-averaged quantities. In the evaluated nuclear data files, there is an energy point that connects the Hauser-Feshbach calculations with the \( 1/v \) cross section. This connection energy is arbitrary but often determined empirically by the average s-wave resonance spacing \( D_0 \). We have found that the connection energy in the evaluated files has a large impact on the calculated MACS for nuclei close to the magic numbers, such as \(^{135}\text{I}\), because relatively large \( D_0 \) pushes the connection point up in the keV range, causing a drastic change in the evaluated capture cross sections. This can be seen in Fig. 3.

In our study, we do not set the connection energy in order to avoid this unphysical behavior in the calculated MACS. Because the Maxwellian distribution drops quickly at low energies, the contribution below 1 keV to MACS is not important. We perform the Hauser-Feshbach calculation from 1 keV, and average the calculated capture cross section over the Maxwellian distribution.

In order to accommodate contributions from the high-energy tail of the Maxwellian distribution, CoH\(^3\) calculates the capture cross section for incident energies ranging from 1 keV to 10 MeV. The cross sections are averaged according to Eq. (1) in the temperature range of interest, \( T = 5 - 30 \) keV. For \(^{135}\text{I}\) we note that statistical methods are employed in the ENDF/B-VII.1 library at 1 keV. We show a comparison of the cross sections, non-averaged and averaged, from ENDF and CoH\(^3\) in Figs. 3 and 4. We can see that when the same general method is applied there is a relevant difference to take into account.

The Hauser-Feshbach-produced MACS in Fig. 4 demonstrates another key aspect of neutron capture cross-sections in astrophysics. While Hauser-Feshbach is applicable in this region, there remain large differences between models due to model parameterizations. Where no experimental information is available, all cross section calculations rely on some phenomenological inputs. These differences can lead to as much as a factor of 20 in the calculated MACS in the case of \(^{135}\text{I}\). A first step in investigating the nuclear uncertainties in the i process is to consider these inter-model differences as systematic uncertainties in Sec. IV.
IV. INTER-MODEL UNCERTAINTIES

Differences between Hauser-Feshbach models can lead to large uncertainties in the calculated neutron capture MACS. As a first step in an uncertainty study we consider the trend of one model to over- or under-estimate the calculated MACS compared to another model. In order to see the effect of these model differences on abundances it is first necessary to determine the reaction rate, $N_A \langle \sigma_\gamma v \rangle$, from the MACS:

$$N_A \langle \sigma_\gamma v \rangle = N_{AvT} \sigma_{\text{Maxw}}$$

$$= N_A \sqrt{\frac{2kT}{\mu}} \sigma_{\text{Maxw}}(T), \quad (2)$$

where $N_A$ is Avogadro’s number.

The nucleosynthetic abundance uncertainties are investigated from the perspective of basic nuclear physics inputs. Therefore, we start from the point of uncertainties generated by the use of two different models for the neutron capture cross section $\sigma_\gamma$ that appears in Eq. (1). For the $i$ process we look at the effect of neutron capture rate uncertainties on 22, unstable fission product nuclei in the region of $^{135}\text{I}$: $^{132-136}\text{Te}$, $^{133-137}\text{I}$, $^{135,137,138}\text{Xe}$, $^{136-139}\text{Cs}$, $^{137,140,141}\text{La}$. Limited experimental information is available on the relevant nuclei, and so $\sigma_\gamma$ is calculated theoretically within the framework of statistical Hauser-Feshbach. The stable isotopes in this region, $^{134,136}\text{Xe}$, $^{136-138}\text{Ba}$ and $^{138,139}\text{La}$, as well as the very long-lived $^{135}\text{Cs}$, are neglected in this study because experimental and evaluated data from KADoNiS [4] are adopted by our nucleosynthesis code [56]. We consider the KADoNiS rates to be the best choice for a given astrophysical neutron capture rate at 30 keV.

We will compare the three Hauser-Feshbach codes CoH$_3$ [51], TALYS 1.4 [52, 53] and NON-SMOKER [54]. NON-SMOKER provides the default neutron capture rates for nuclei in the region of interest for these simulations. It is commonly employed by the astrophysics community through its use for theoretical rates in the JINA REACLIB [2] library.

The MACS produced by TALYS 1.4 under-estimates the MACS from NON-SMOKER on average by 4% in this region. CoH$_3$, on the other hand, over-estimates the MACS from NON-SMOKER on average by a factor of about 1.4. However, this trend is not always maintained. Some exceptions are shown in Fig. 5 comparing the neutron capture MACS on a log scale as a function of temperature from the three models for three unstable nuclei in the region of interest: $^{132}\text{Te}$, $^{135}\text{I}$ and $^{140}\text{Ba}$. These nuclei show how the differences among the models cannot be accounted for by a single constant offset, despite a general trend. We therefore expect that a systematic application of uncertainty for each of the 22 nuclei in question which accurately reflects the large model differences is necessary to fully represent the effect of neutron capture uncertainties on the $i$-process abundances.

For each of the 22 nuclei we use the neutron capture
rates from the different models to investigating the systematic uncertainty amongst them. The effects of this uncertainty are demonstrated on observable elemental ratios. Figure 6 plots the effects of the uncertainty arising from different models on the [Ba/La] and [La/Eu] ratios. Each point represents the ratio of elements at a different time within the simulation, where the left most point is the earliest time (about $t = 1.59 \times 10^{-4}$ years) and proceeding along the curve in increments of about $8 \times 10^{-6}$ years. In Fig. 6, the black curve shows the evolution of these ratios using the default NON-SMOKER rates. The red and blue curves show the element ratio evolution when using the neutron capture rates from CoH$_3$ and TALYS 1.4, respectively.

Figure 6 shows the effect of the systematic differences in neutron capture rates among the three Hauser-Feshbach models. Between NON-SMOKER and CoH$_3$ (TALYS 1.4) differences in capture rates can lead to as much as a factor of 22 (47) in the [Ba/La] ratio, and 1.3 (19) in the [La/Eu] ratio. The differences change not only the value of the [Ba/La] and [La/Eu] ratios, but the shape of their evolution. The evolution of the ratios for the CoH$_3$ and TALYS 1.4 rates compared to each other and to NON-SMOKER demonstrate that the neutron capture rates do not simply cause horizontal or vertical off-sets to the element ratio curves.

We are interested in the role of correlated nuclear physics uncertainties on the i-process abundances. In order to investigate this we look at the application of neutron capture rates from different models for all 22 nuclei in the region of the neutron shell closure $N = 82$, compared to changing only the bottle-neck neutron capture cross section on $^{135}$I. The comparison is shown in Fig. 7. While one might expect $^{135}$I neutron capture rate to dominate the changes to the [Ba/La] and [La/Eu] ratios, the effects of the remaining 21 neighbouring nuclei is important to consider. Using different models for only the bottle-neck does change the shape and values of the element ratio evolution for CoH$_3$ compared to NON-SMOKER. Yet application of these models to all 22 nuclei results in more drastic changes to the [Ba/La] and [La/Eu] ratios, as well as significant changes to the shape of the evolution.

On the other hand, the comparison between NON-SMOKER and TALYS 1.4 seems to give a different result. In the lower panel of Fig. 7 there is not as significant a difference between using TALYS 1.4 for only neutron capture on $^{135}$I (red “x”) to using CoH$_3$ for the full set of 22 nuclei (red triangle). Bottom: Same as top panel, but using TALYS 1.4. In both cases the elemental ratios from the default NON-SMOKER rates are shown in black.

FIG. 6: (Colour online) Comparison of the [Ba/La] and [Eu/La] ratios over time when using the default NON-SMOKER (black), CoH$_3$ (red) and TALYS 1.4 (blue) models.

FIG. 7: (Colour online) Top: Compares the effects on the [Ba/La] and [La/Eu] ratios when using CoH$_3$ for only the bottle-neck nucleus $^{135}$I (red “x”) to using CoH$_3$ for the full set of 22 nuclei (red triangle). Bottom: Same as top panel, but using TALYS 1.4. In both cases the elemental ratios from the default NON-SMOKER rates are shown in black.
factor of four on neutron capture reactions, which corresponds to the difference between the $^{135}$I neutron capture rate in CoH$_3$ and NON-SMOKER. We plot in Fig. 8 the element ratios resulting from a constant factor of four applied to all 22 nuclei around $^{135}$I, as well to only the bottle-neck neutron capture on $^{135}$I. Applying the offset to only $^{135}$I reproduces a similar behaviour seen in the upper panel of Fig. 7 as we would expect. However, the constant factor of four results in an even more drastic change to both the [Ba/La] and [La/Eu] values due to its simplicity, numerical stability and low computational cost. Equation (3) is then used in the (now correlated) random sampling of parameter sets, by projecting parameter correlations within the model. This is achieved by generating a prior correlation matrix in a linearization method via the Jacobian of the model with respect to the relevant parameters $^{58-61}$:

\[ V_{ij} = \langle (\sigma_{ik} - \sigma_{i0})(\sigma_{jk} - \sigma_{j0}) \rangle \quad i, j = 1, l \quad (3) \]

where $k$ is the number of Monte Carlo histories and $k = 0$ uses the optimized parameter set $p_0$. The uncertainty in the simulation then goes as $1/\sqrt{k}$.

The Monte Carlo method used in this work generates the random parameter sets in a manner that accounts for parameter correlations within the model. This is achieved by generating a prior correlation matrix in a linearization method via the Jacobian of the model with respect to the relevant parameters $^{58-61}$:

\[ V_{ij}^m = \chi^2(J(p_0)^T J(p_0))^{-1} \quad (4) \]
\[ C_{ij}^m = \frac{V_{ij}^m}{\sqrt{V_{ii}^m V_{jj}^m}} \quad (5) \]

where $V_{ij}^m$ and $C_{ij}^m$ are the prior model covariance and correlation matrices, respectively. The covariance matrix in Eq. (4) depends on the root-mean-square variation, $\chi^2$, that results from fitting the optimal parameter set $p_0$. We note that because we employ the correlation matrix $C_{ij}^m$, there is no longer a dependency on $\chi^2$. Other methods for approximating a model covariance exist, however this is the preferred method of Refs. $^{58, 59}$ due to its simplicity, numerical stability and low computational cost. Equation (5) is then used in the (now correlated) random sampling of parameter sets, by projecting appropriate Gaussian-distributed random numbers onto the correlated space. This allows for a first-order approximation to the prior covariance matrix, rather than assuming a purely diagonal prior covariance as is frequently used $^{57, 61}$.

While the statistical Hauser-Feshbach methods employ a large number of parameters that may be varied, it is sufficient to perform a Monte Carlo covariance analysis on a small set of the most crucial parameters. The set of seven parameters varied in this analysis are related to the optical model, level density parameters, and the average $\gamma$-ray width. CoH$_3$ uses the global optical model parameterization provided by Koning and Delaroche $^{62}$. We adjust the real potential depth, $V_r$, and imaginary surface potential depth, $W_p$. These potential depths have a reported uncertainty of 2% and 10%, respectively. We also adjust the real potential radius, $r_V$, and imaginary surface potential radius, $r_D$, within their reported uncertainty of 0.001 fm for both.

V. SYSTEMATIC AND STATISTICAL UNCERTAINTY

To consider the effects of detailed statistical correlations on final abundances we now look specifically at a single Hauser-Feshbach model. We employ the Los Alamos National Laboratory (LANL) in-house statistical Hauser-Feshbach code CoH$_3$ in calculating the $(n, \gamma)$ cross sections in the region of $N = 82$. However, within the statistical method large uncertainties still exist. An analysis of the uncertainty in the calculated capture cross sections is performed via a Monte Carlo covariance analysis $^{57}$.
In addition to the four optical model parameters listed above, we adjust two parameters of the Gilbert-Cameron level density model [63]. The pairing energy, $\Delta$, and the level density parameter, $a$, are adjusted within an uncertainties of 30% and 2.4%, consistent with systematics reported in Ref. [63]. The last parameter is the level density parameter, $\gamma$. All seven parameters are varied simultaneously in the Monte Carlo fashion described above, where random variations are generated from a Gaussian distribution with a standard deviation equal to the parameter’s reported uncertainty. Correlations amongst all the parameters within the model are accounted for via Eq. (3) and the above described projection.

These parameters are chosen because the model and underlying physics depends sensitively on their value. Figure 9 shows the distribution of $^{135}$I neutron capture cross sections at 30 keV in 0.1 mb bins. The variance of this distribution, given by Eq. (3), provides the uncertainty in the cross section at this energy.

In Fig. 10 we show the percent uncertainty in the $^{135}$I capture cross section as a function of incident neutron energy which results from the Monte Carlo variation. The variance of this distribution provides the uncertainty in the calculation.

In Fig. 10 we show the percent uncertainty in the $^{135}$I capture cross section as a function of incident neutron energy from the Monte Carlo covariance analysis. As one can see, the model uncertainty is not negligible and provides a necessary constraint on the uncertainties present in a crucial astrophysical reaction. The percent uncertainty is shown to go above 100% at incident energies higher than 1.5 MeV. This comes from the long tail in the asymmetric distribution seen in Fig. 9 where the calculation of the percent uncertainty assumes a Gaussian (symmetric) probability density function via Eq. (3) as pointed out in Ref. [64]. As captured on excited states of the target nucleus must be considered in an astrophysical environment. Therefore, sensitivity studies of nucleosynthesis on MACS are not accurately bounded by the uncertainty in experimental results on only ground state targets and it becomes necessary to use the model uncertainty as the appropriate lower bound [64].

A. Propagating Uncertainties

The goal is to propagate the uncertainties in the Hauser-Feshbach parameter set not just to the cross section, but through to the final abundance of the $i$ process. In order to achieve this, these uncertainties must be propagated through the MACS, rates and the nucleosynthesis simulation. In all steps, a stochastic method is employed allowing us to directly include all non-linear effects.

The Monte Carlo propagation of the Hauser-Feshbach parameter uncertainties through the MACS calculation is straightforward. The capture cross sections at $l$ energies generated by the random simulation of model input parameters is used directly within Eq. (1) to generate MACS for each Monte Carlo history. Using the same method of Eq. (3) we can statistically determine the covariance matrix for the MACS at the various stellar temperatures,

$$V_{ij}^{\text{Maxw}} = \langle (\sigma_{\text{Maxw},k}(T_i) - \sigma_{\text{Maxw},0}(T_i)) \times (\sigma_{\text{Maxw},k}(T_j) - \sigma_{\text{Maxw},0}(T_j)) \rangle \quad i, j = 1, M,$$

where $M$ defines the number of temperatures, $T$, considered. The same can be applied to investigate the covariance matrix amongst various isotopes with $\sigma_{\text{Maxw},k}(T_i) \rightarrow \sigma_{\text{Maxw},k}(N_i, Z_i, T_i)$.

With the stochastic distribution of MACS available it is possible to propagate these uncertainties through the rate and, subsequently, the nucleosynthesis simulations. We choose to consider the neutron capture at 30 keV.
TABLE I: Percent uncertainty in the Hauser-Feshbach neutron capture cross section and MACS at 30 keV for 22 unstable nuclei in the region of $N = 82$.

| Isotope | % Unc. $\sigma_\gamma$ (30 keV) | % Unc. $\sigma_{Maxw}$ (30 keV) |
|---------|----------------------------------|----------------------------------|
| $^{132}$Te | 27 | 23 |
| $^{133}$Te | 43 | 38 |
| $^{134}$Te | 21 | 23 |
| $^{135}$Te | 45 | 51 |
| $^{136}$Te | 26 | 24 |
| $^{133}$I | 22 | 27 |
| $^{134}$I | 8 | 28 |
| $^{135}$I | 28 | 37 |
| $^{136}$I | 31 | 34 |
| $^{137}$I | 54 | 45 |
| $^{135}$Xe | 11 | 22 |
| $^{137}$Xe | 73 | 34 |
| $^{138}$Xe | 23 | 22 |
| $^{136}$Cs | 40 | 46 |
| $^{137}$Cs | 11 | 30 |
| $^{138}$Cs | 24 | 44 |
| $^{139}$Cs | 90 | 29 |
| $^{139}$Ba | 6 | 30 |
| $^{140}$Ba | 30 | 22 |
| $^{137}$La | 43 | 40 |
| $^{140}$La | 45 | 41 |
| $^{141}$La | 44 | 38 |

because it is the maximum applicable energy for stellar reactions in this scenario. Where the uncertainty is a monotonically increasing function of energy (see Fig. [10]) this provides the greatest uncertainty for each reaction, giving the least optimistic perspective of abundance uncertainties.

B. Correlated vs. Uncorrelated Uncertainties

The neutron flow shows a bottle-neck at $^{135}$I. We stochastically propagate uncertainties from neutron capture reactions on 22 nuclei in the region of $^{135}$I through the stellar neutron capture rate of Eq. (2) and on to the final abundances of the $i$ process. We compare the effects of independent (uncorrelated) changes to $^{135}$I neutron capture and correlated changes to neutron capture rates on all 22 nuclei in the region on final stellar abundances. Via Eq. (3) we calculate the percent uncertainty in the neutron capture cross section for each of the 22 nuclei in the region of $^{135}$I, displayed in Table I.

The neutron capture cross section uncertainties at 30 keV are as low as 6% in one case ($^{139}$Ba), but in general are a factor of two or more. Because the MACS involves a folding over capture cross sections at several energies it is not surprising that the range of uncertainty is much smaller (right-most column of Table I).

Whereas global parameterization may be very well determined within the Hauser-Feshbach model at 30 keV for certain nuclei, the Maxwellian average for a range of incidence neutron energies from the statistical method produces similar uncertainties for each isotope. We note that these uncertainties arise from the statistical method with which we calculated the cross sections, and does not signify those uncertainties that are present amongst different models. The global uncertainties amongst models are significantly larger. However, by constraining our focus to those uncertainties within a single model we are able to address the statistical correlations amongst neutron capture rates.

In order to quantify the uncertainty in the final abundance, the Monte Carlo history rates are propagated directly in the nucleosynthesis simulations. The direct propagation contains all correlations from the model. In the correlated case Monte Carlo histories are propagated for all 22 nuclei around $N = 82$, whereas the uncorrelated case only propagates histories for $^{135}$I. We perform the same statistical uncertainty analysis on the abundances as with the neutron capture cross sections and MACS. From all $k$ Monte Carlo histories we construct the covariance matrix similarly to Eqs. (4) and (5).

$$V_{ij}^{\text{elem}} = \langle (X_{ik} - \bar{X}_i)(X_{jk} - \bar{X}_j) \rangle \quad i, j = 1, \mathcal{N},$$

where $\mathcal{N}$ is the total number of elements in the nucleosynthesis simulation and $X_i$ is the mass fraction of the $i$th element. We let $k = 0$ be the default, NON-SMOKER rate-based, abundances from NuGrid in order to include the systematic uncertainty present between CoR3 and NON-SMOKER codes. This gives us a picture of the full systematic and statistical uncertainties. The diagonal elements of the covariance matrix $V_{ii}^{\text{elem}}$ provide the uncertainty bounds on each elemental abundance where

$$V_{ii}^{\text{elem}} = (\delta X_i)^2$$

and $\delta X_i$ is the uncertainty in the $i$th elemental abundance.

Figure [11] shows the final abundance as mass fraction of the star for relevant elements in the uncertainty study, where all isotopes have been allowed to decay to stability. The error bars indicate the uncertainty resulting from a Monte Carlo propagation of correlated uncertainties in neutron capture rates. One immediately notices the large abundance uncertainties which result from the underlying nuclear physics, even on elements no included in the study (i.e. $Z > 57$). Yet elements Te and I show very little uncertainty (factors of $4 \times 10^{-3}$ and $6 \times 10^{-3}$ uncertainty, respectively), demonstrating the role of coupling to the neutron flow on final abundance uncertainties.

Figure [12] provides an initial insight into the importance of correlated uncertainties for elemental abundances. The relative error profile in abundances due to uncorrelated changes to the $^{135}$I capture rate shows
FIG. 11: (Colour online) Elemental abundances given as mass fraction of star for the i process. Error bars indicate uncertainty in elemental abundances from correlated changes to neutron capture rates. Uncertainties are propagated using a Monte Carlo method.

FIG. 12: (Colour online) Comparison of fully correlated relative uncertainty for the 22 isotopes studied to uncorrelated uncertainty resulting from changes in $^{135}$I($n, \gamma$) alone.

a peak at Xe and then remains constant for elements larger than Ba. These uncertainties are a factor of two, consistent with expectations on uncertainties in Hauser-Feshbach models. However, we see unrealistically low uncertainties for Te, I and Cs (factors of $5 \times 10^{-3}$, $7 \times 10^{-3}$ and $6 \times 10^{-3}$, respectively).

Correlated neutron capture uncertainties result in greater uncertainties in abundances on average. Additionally, there is more variation in the uncertainty across elements, particularly above Ba where the uncorrelated case returns nearly constant uncertainties. Most notably in the figure, we see a large spike at Cs (factor of about 3.5) for the correlated case, resulting from decay of $^{133}$Te and $^{131}$I whose neutron capture uncertainties are only included in the correlated case.

FIG. 13: (Colour online) The evolution of the relative uncertainty (on log-scale) in $[\text{Ba/La}]$ and $[\text{La/Eu}]$ ratios over time resulting from both the correlated and uncorrelated Monte Carlo studies.

C. Importance of Statistical Correlation in Nucleosynthesis

The results presented in Figs. 11 and 12 show that neutron capture cross section uncertainties can lead to noticeable uncertainties in the final elemental abundances. Including uncertainties from a larger range of isotopes more accurately represents the overall nuclear physics uncertainty and allows one to move beyond initial sensitivity studies. In the case of the i process, correlations in neutron capture uncertainties play a meaningful role in final abundances. Figure 12 has shown a more complex uncertainty is present across elements when correlated uncertainties are used. Yet the inclusion of correlated uncertainties is further demonstrated by considering again the ratio of observable elements.

In Fig. 13 we plot the relative uncertainty of elemental ratios $[\text{Ba/La}]$ and $[\text{La/Eu}]$ over time, with uncertainties from both correlated and uncorrelated propagation of neutron capture rate uncertainties. The uncertainties shown here are consistent with what we might expect from the differences between CoH$_3$ and NON-SMOKER seen in Fig. 6 when including both systematic and statistical uncertainties. The evolution in the uncertainties in elemental ratios elicits some behaviour of correlated uncertainties in neutron capture rates hinted at in Fig. 12. Over time the uncertainties change for both ratios, corresponding to variations in the influence of neutron capture on isotope production with the changing stellar environment. In the nucleosynthesis calculations done with the 1-zone trajectory introduced in Sec. II at about $t = 5 \times 10^{-4}$ years the first neutron flux hits the region of $^{135}$I. A major abundance flow continues here in the following trajectory evolution.

For the $[\text{Ba/La}]$ ratio we see that the uncorrelated case is consistently lower than the correlated case. In earlier
times (about $t = 3.4 - 6 \times 10^{-4}$ years) we see some oscillations in the uncorrelated uncertainty of the $[\text{Ba/La}]$ ratio, with the uncertainty becoming as low as a factor of 0.01. Such a low uncertainty is about a factor of 30 lower than the correlated case, and is lower than one might reasonably expect. However, this lower uncertainty is an artifact of the uncorrelated uncertainty study. As the uncertainties in two quantities approach a correlation of one the relative uncertainty in their ratio approaches zero:

$$\frac{\text{var}(A/B)}{(A/B)^2} = \frac{\text{var}(A)}{A^2} + \frac{\text{var}(B)}{B^2} - 2\frac{\text{cov}(A,B)}{AB}. \quad (9)$$

In the uncorrelated case $^{135}$I acts as a single source of uncertainty causing an artificially high correlation in heavier element production. More interestingly, the oscillations indicate a strong coupling to the stellar environment which influences the level of this artificially high correlation. Thus, we see the greatest limitation of applying only a single rate uncertainty is in describing elemental ratios. Inaccurately representing the correlation in elemental production with uncorrelated nuclear physics uncertainties result in uncertainties wrongly appearing to cancel, a la Eq. (9).

For the $[\text{La/Eu}]$ ratio we see a slightly different situation. The correlated case tends to have a higher uncertainty than the uncorrelated case. However, we see a decrease of about an order of magnitude in the correlated uncertainty at about $t = 15 \times 10^{-4}$ years, below the uncorrelated uncertainty. During this time, the uncorrelated uncertainty remains nearly constant. This indicates a correlation in the production of La and Eu that occurs in the stellar environment. However, this production correlation is only captured in when correlated changes to neutron capture rates are used in the uncertainty study. Uncorrelated changes to only $^{135}$I do not reproduce this production correlation. Both the correlated and uncorrelated cases have the general shape in the uncertainty curve in the last $20 \times 10^{-4}$ years, for both the $[\text{Ba/La}]$ and $[\text{La/Eu}]$ ratios.

VI. CONCLUSIONS

While Hauser-Feshbach is a critical theory for astrophysical neutron capture rates, large differences exist amongst different codes. Investigating the systematic effects on elemental abundances from the codes NON-SMOKER, CoH$_3$ and TALYS 1.4 has shed light on the role of neutron capture uncertainties in the i process beyond single reaction sensitivity tests. Even with a bottleneck reaction, such as neutron capture on $^{135}$I, the uncertainties present in surrounding neutron capture rates play a significant role. Furthermore, in order to maintain consistency between any two Hauser-Feshbach codes it is not sufficient to apply a single offset to all reaction rates indiscriminately. Rather, one must account for the systematic differences between codes.

Looking beyond systematics, we have provided true error bars on final elemental abundances in the i process by performing a Monte Carlo propagation of nuclear physics uncertainties through the stellar simulation, beginning with uncertainties in the parameters of the Hauser-Feshbach code CoH$_3$. By performing our statistical comparison directly to abundances using NuGrid's default NON-SMOKER rates we are able to describe statistical and systematic uncertainties.

The uncorrelated changes to a single neutron capture rate inaccurately describe the elemental abundance correlations and uncertainties. We conclude this with the assumption that including more physics (i.e. more reaction rate uncertainties) more accurately describes the complete physics of the system. This is expected, and we see from Figs. 12 and 13 that the role of correlations is significant. The uncorrelated case tends to under-estimate the uncertainty in final elemental abundances, except in early times where we see an artificial oscillation in production correlations. Elemental abundance ratios are also key observables and their uncertainty further indicates the importance of correlations in reaction rate uncertainties. Within a given astrophysical model not including reaction correlations leads to an under-estimation of the element ratio uncertainties. Furthermore, this gives insight into the influence of reaction rate uncertainties and correlations on elemental abundance correlations.

Including uncertainties from 22 neutron capture rates leads to noticeable differences in elemental abundance uncertainties over changes to a single reaction rate. From Fig. 13 we can already see the complex, dynamic environment present in fully propagating nuclear physics uncertainties through to elemental abundances. In particular, we show that in i-process conditions the uncertainty on nucleosynthesis theoretical predictions for the $[\text{Ba/La}]$ and $[\text{La/Eu}]$ ratios may change significantly by using different Hauser-Feshbach models. The sources of these differences need to be analyzed in detail. $[\text{Ba/La}]$ and $[\text{La/Eu}]$ are indicative observables to distinguish for instance between CEMP-s, CEMP-r and CEMP-r/s stars, and therefore provide fundamental insights to analyze the nature of CEMP-r/s stars. We have shown that the $[\text{La/Eu}]$ is changing by about 0.5 dex by using different Hauser-Feshbach models, while the $[\text{Ba/La}]$ by up to 1 dex. In particular, using the NON-SMOKER reaction rates in our simple 1-zone model the i-process results overlap with the observed range of CEMP-r/s stars. In this scenario at least a significant fraction of CEMP-r/s stars are instead CEMP-i stars, according to the conclusions of Herwig et al. [22], and the primary star responsible for the carbon and i-process enrichment might be a super-AGB companion. Using TALYS rates, i-process simulations covered the observed range of $[\text{La/Eu}]$ but does not cover the entire range of $[\text{Ba/La}]$. Finally, using CoH$_3$ the i-process signature is quite similar to an s-process signature for these elements, and therefore is not able to explain the CEMP-r/s abundances spread with the simple 1-zone trajectory. This shows that while robust
i-process predictions depend on the details of the hydrodynamics simulations to correctly follow to H ingestion event (e.g., Herwig et al. \cite{2002ApJ...573..996H}, Stancliffe et al. \cite{2010MNRAS.403..326S}, Woodward et al. \cite{2011MNRAS.412.2846W}), there are critical nuclear uncertainties that need to be addressed in the neutron capture flow region typical of the i process.

Including uncertainties from more reaction rate correlations will lead to even further changes to the uncertainty. There remain open questions on the role of cross-region correlations, as well as including more than neutron capture rates. In exotic neutron capture environments, competition with beta-decay is likely to introduce crucial correlations.

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\[(n,\gamma)\text{ MACS (mb)}\]

| T (keV) | \(^{137}\text{Cs NON-SMOKER}\) | \(^{137}\text{Cs CoH3}\) | \(^{137}\text{Cs TALYS 1.4}\) |
|---|---|---|---|
| 5 | | | |
| 10 | | | |
| 15 | | | |
| 20 | | | |
| 25 | | | |
| 30 | | | |