Extensive study of nuclear uncertainties and their impact on the r-process nucleosynthesis in neutron star mergers

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ABSTRACT

Theoretically predicted yields of elements created by the rapid neutron capture (r-) process carry potentially large uncertainties associated with incomplete knowledge of nuclear properties as well as approximative hydrodynamical modelling of the matter ejection processes. We present an in-depth study of the nuclear uncertainties by systematically varying theoretical nuclear input models that describe the experimentally unknown neutron-rich nuclei. This includes two frameworks for calculating the radiative neutron capture rates and six, four and four models for the nuclear varying theoretical nuclear input models that describe the experimentally unknown neutron-rich nuclei. The impact of nuclear uncertainties on the r-process abundance distribution and early radioactive heating rate is found to be modest (within a factor $\sim 20$ for individual $A > 90$ nuclei and a factor 2 for the heating rate), however the impact on the late-time heating rate is more significant and depends strongly on the contribution from fission. We witness significantly larger sensitivity to the nuclear physics input if only a single trajectory is used compared to considering ensembles of $\sim$200-300 trajectories, and the quantitative effects of the nuclear uncertainties strongly depend on the adopted conditions for the individual trajectory. We use the predicted Th/U ratio to estimate the cosmochronometric age of six metal-poor stars to set a lower limit of the age of the Galaxy and find the impact of the nuclear uncertainties to be up to 2 Gyr.

Key words: Nuclear reactions, nucleosynthesis, abundances – Neutron star mergers

1 INTRODUCTION

Through a series of neutron captures and $\beta$-decays on light nuclei, the rapid neutron capture process (or r-process) can explain the production of about 50% of the stable (and some long lived) neutron-rich nuclides heavier than iron, as initially proposed by Burbidge et al. (1957); Cameron (1957). Since then and until a few years ago, the astrophysical site(s) of the r-process remained essentially unknown and most of the r-process studies (for reviews, see, e.g., Arnould et al. 2007; Arnould & Goriely 2020; Cowan et al. 2021) relied on simple assumptions about the physical environment and equations for the abundance evolution. Recently, our understanding of the astrophysical site for the r-process and the nucleosynthesis has improved drastically both in terms of observational data but also due to computational advancements of site-specific simulations. Currently, the most sophisticated and realistic r-process calculations rely on advanced hydrodynamical simulations which dictate the conditions of the astrophysical environment where the nucleosynthesis occurs, and a full nuclear reaction network with regularly improved nuclear physics input is applied in a post-processing step (due to computational constraints). This way the r-process calculations are site dependent, i.e. the results are sensitive to the astrophysical scenario adopted for the calculations.

Until a decade ago, the neutrino-driven wind launched during a core-collapse supernova (CCSN) was a very popular candidate for the r-process site. However, the conditions required for a successful r-process have not been obtained in the most sophisticated existing models (e.g., Witti et al. 1994; Hüdepohl et al. 2010; Mirizzi et al. 2016; Roberts et al. 2010; Fischer et al. 2010; Wanajo et al. 2018, and references therein). The focus shifted towards binary neutron star (NS) mergers after hydrodynamical models managed to demonstrate that a significant amount of material ($10^{-3} - 10^{-2}M_\odot$) can become unbound in the dynamical phase of NS-NS mergers (e.g., Ruffert et al. 1997; Ruffert & Janka 1999; Freiburghaus & Rosswog 1999; Rosswog et al. 1999; Ruffert & Janka 2001; Janka & Ruffert 2002; Oechslin et al. 2007; Goriely et al. 2011; Hotokezaka et al. 2013; Bauswein et al. 2013). The final observational confirmation that r-process material is synthesized in NS-NS mergers came in 2017 with the first gravitational wave detection from a NS-NS merger, GW170817 (e.g., Abbott et al. 2017a) accompanied by an electromagnetic signal, AT2017gfo (Abbott

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et al. 2017b; Kasen et al. 2017; Watson et al. 2019). However, it is not observationally settled yet whether binary NS mergers can also produce the heaviest of the solar r-process elements and whether they are the only r-process site, or if other sites contribute to the Galactic enrichment. For example, outflows associated with jets in core-collapse supernovae or from accretion tori around black holes forming in collapsing, rapidly rotating massive stars, so-called collapsars (MacFadyen & Woosley 1999), were considered in numerous papers (e.g., Cameron 2001, 2003; Winteler et al. 2012; Nishimura et al. 2015; Mösta et al. 2018; Siegel et al. 2019; Grimmett et al. 2020; Just et al. 2021a; Reichert et al. 2021; Cowan et al. 2021; Just et al. 2022; Reichert et al. 2022; Siegel 2022). In particular, the question of the earliest possible onset of r-process nucleosynthesis from NS-NS mergers during the galactic chemical evolution comes with significant uncertainties. One problem may be that the time required to form the first NS binary systems plus their in-spiral phase before merging is too long to explain the presence of Eu in metal-poor halo stars, and therefore another r-process site might be needed (Hotokezaka et al. 2018; Côté et al. 2019). This conclusion, however, has been weakened by several chemical evolution models (e.g., Shen et al. 2015; Dvorkin et al. 2020; van de Voort et al. 2020, 2022). More work in this regard is required to settle this debate.

During and shortly after the merging, the NS-NS system undergoes several mass ejection phases (see Fig. 1) which depend on the binary system parameters and the properties of the nuclear equation of state (EoS). In the first phase, matter is ejected dynamically both from the tidal tails of the NSs after they interact as well as from the shock-heated material originating from the contact interface. The ratio between the cold tidal and hot shocked ejecta mainly depends on the mass originating from the contact interface. The ratio between the nuclear equation of state (EoS). In the first phase, matter undergoes several mass ejection phases (see Fig. 1) which depend on the binary system parameters and the properties of the nuclear EoS, where the relative amount of cold tidal ejecta and stiffer EoSs (Bauswein et al. 2013). In addition, it was discussed already in early papers (Ruffert et al. 1997; Ruffert & Janka 2001) that the inclusion of weak nucleonic reactions of electron neutrinos ($\nu_e$) with free neutrons ($n$) and electron antineutrinos ($\bar{\nu}_e$) with free protons ($p$) as well as their inverse reactions

\[
\nu_e + n \rightarrow p + e^-, \quad \bar{\nu}_e + p \rightarrow n + e^+
\]

might significantly change the initial composition of the ejecta. Indeed, this was later shown by numerical modelling (e.g., Wanajo et al. 2014; Goriley et al. 2015; Martin et al. 2018; Radice et al. 2016; Foucart et al. 2016; Kullmann et al. 2021, and references therein). Since the r-process nucleosynthesis is very sensitive to the initial composition, in particular to the neutron richness of the material, it is critical to base r-process calculations on hydrodynamical simulations which include such neutrino reactions.

Similar to NS-NS mergers, a significant amount of neutron-rich material can also be ejected from NS-black hole (BH) mergers (e.g., Janka et al. 1999; Etienne et al. 2008, 2009; Kyutoku et al. 2013; Bauswein et al. 2014; Just et al. 2015a; Kiuchi et al. 2015; Fernández et al. 2017, 2020; Krüger & Foucart 2020) so that they are also viable candidates for the r-process site. The evolution from two orbiting, in-spiralling compact objects to a BH or a long-lived NS remnant depends on the initial conditions of the system. In NS-BH mergers with sufficiently small BH masses and in NS-NS mergers with sufficiently high total masses and/or a sufficiently soft EoS, a BH-torus system is formed right after the merger. Alternatively, if the NS remnant can be stabilized against a prompt collapse in a NS-NS merger, it will evolve as a (hyper- or super-) massive NS and either undergo a delayed collapse after some time or remain indefinitely stable. In both kinds of remnants, BH-torus and massive NS systems, material can be expelled due to turbulent viscosity, neutrino heating, or magnetic-fields effects (e.g., Metzger & Fernández 2014; Siegel & Metzger 2018; Hosseini Nouri et al. 2018; Christie et al. 2019; Miller et al. 2019; Fernández et al. 2019; Fujibayashi et al. 2018; Fujibayashi et al. 2020a,b; Perego et al. 2014; Perego et al. 2021; Just et al. 2015a; Just et al. 2022; Pahlman & Fernández 2022).

Great efforts have been put into hydrodynamical simulations of different NS-NS or NS-BH merger configurations in the last decade. An important goal for the community is to develop astrophysically consistent models which can estimate the total amount of ejecta, either by combining models consistently, or ideally by covering the entire evolution of the merging system. Recently, improved models including fully relativistic approaches have managed to cover the dynamical phase and the late-time evolution of the remnant and secular ejecta (Kawaguchi et al. 2021; Hayashi et al. 2021). Note that the NS-NS simulations of Kawaguchi et al. (2021) involve a mapping between different codes; see also Just et al. (2015a) for an early attempt to combine different ejecta components in a “system-preserving” (thus attempting consistency) manner. However, due to computational constrains, most models only cover one phase of the evolution, i.e. either the dynamical or the secular phase.

In this work, we will base our r-process nucleosynthesis calculations on state-of-the-art hydrodynamical simulations that estimate the dynamical ejecta of two NS-NS and one NS-BH mergers and, separately, two BH-torus simulations of the post-merger phase. By combining the appropriate hydrodynamical models for the dynamical and secular ejecta, we will estimate the nucleosynthesis composition of the total ejecta.

After high resolution spectra became available for metal-poor stars, it has become possible to derive the abundances of long-lived radioactive elements such as thorium and uranium in stellar spectra of r-process enhanced metal-poor stars. This has opened the doors for an independent age-dating method of individual stars and, therefore, also lower limits on the age of our Galaxy. The method, called cosmochronometry (Butcher 1987), relies on the known radioactive decay time (i.e. half-life) of long-lived radioactive nuclei, and the theoretical prediction of the initial abundance (before decay) of the involved nuclei. By combining the known radioactive decay time for $^{238}$U and $^{232}$Th of $\tau(U) = 6.54$ Gyr and $\tau(Th) = 20.27$ Gyr, respectively, an age estimate of the star ($t^{\star}_{U, Th}$) can be calculated from

\[
\log \left( \frac{\text{Th}}{U} \right)_{\text{obs}} = \log \left( \frac{\text{Th}}{U} \right)_{\text{r}} + \log \left( e \left( \frac{1}{\tau(U)} - \frac{1}{\tau(Th)} \right) \right) \times t^{\star}_{U, Th}
\]

(2)

where (Th/U)$_{\text{obs}}$ and (Th/U)$_{\text{r}}$ are the observed and model-dependent r-process abundance ratios, respectively, of $^{232}$Th and $^{238}$U (after decay of their shorter-lived isotopes) taken directly from the r-process calculations. Other cosmochronome-
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In addition to the astrophysical modelling uncertainties, r-process nucleosynthesis calculations rely on nuclear models and experimental data for about 5000 nuclei, of which only a tiny fraction is experimentally known. Thus, theoretical models are crucial to predict fundamental nuclear properties such as nuclear masses, α- and β-decay rates, radiative neutron capture rates and fission probabilities. Despite much progress, these nuclear models are still affected by a variety of uncertainties, in particular for the complex description of exotic neutron-rich nuclei. In addition to the radiative neutron captures and the reverse photodisintegrations, all charged-particle fusion reactions on light and medium mass elements and β-delayed neutron emission probabilities become important when the statistical equilibrium freezes out. If the r-process reaches the fissionable region, fission processes such as neutron-induced, spontaneous and β-delayed fission, together with the corresponding fission fragment distribution have to be taken into account for all fissioning nuclei. Previous works have shown that the nuclear uncertainties can significantly affect the results for the r-process abundance (e.g., Caballero et al. 2014; Mendoza-Temis et al. 2015; Eichler et al. 2015; Goriely 2015b; Martin et al. 2016; Liddick et al. 2016; Mumpower et al. 2016; Nishimura et al. 2016; Bliss et al. 2017; Denissenkov et al. 2018; Vassh et al. 2019; Nikas et al. 2020; Sprouse et al. 2020; McKay et al. 2019; Giuliani et al. 2020) and, therefore, for the radioactive heating rate that gives rise to the observable kilonova emission (e.g., Rosswog et al. 2017; Zhu et al. 2018; Wu et al. 2019; Even et al. 2020; Zhu et al. 2021; Barnes et al. 2021). However, the conclusions of these studies may change with, for example, the inclusion of nucleonic weak interactions in the dynamical ejecta or the ability for the r-process to reach the fissionable region, as discussed in Lemaitre et al. (2021); Kullmann et al. (2021).

To estimate the sensitivity of the r-process nucleosynthesis yields to the nuclear input, many studies up to now have been using Monte Carlo type simulations (e.g., Mumpower et al. 2016; Nikas et al. 2020). In this approach, reaction or decay rates are classically modified in a given range, independently of the changes of other reactions, and these modified sets of reactions are used to compute the nucleosynthesis. This approach is correct, if rates are uncorrelated; this may be the case in particular for experimentally determined cross sections or temperature-dependent β-decay rates, for which the properties are intrinsic to each specific case and do not affect rates of neighbouring nuclei. However, in the case of theoretically derived rates, those are predicted by a given model that defines the correlations between all reactions, either locally (e.g., by modifying a given structure property of a specific nucleus) or globally (e.g., by changing the model adopted to describe the structure properties of interacting nuclei or the interaction with nucleons or photons). More specifically, changing a specific theoretical rate by a given factor without affecting other rates, either locally or globally, can hardly be justified. For example, if a rate is uncertain because of the still unknown mass of the target nucleus, this will affect the production as well as destruction rates of this nucleus through a modification of the corresponding Q-value. Consequently, none of the (destruction or production) rates can be changed independently from the other. Similarly, theoretical rates are correlated by the underlying reaction model and the many nuclear models adopted to describe the ingredients of the reaction model, such as nuclear masses, nuclear level densities, photon strength functions, and the optical potentials. With this in mind, we will study the uncertainties related to theoretical nuclear models on the r-process nucleosynthesis by varying the input systematically between global models that have been adjusted on the full set of available experimental data.

This paper is organized as follows: In Sec. 2 we introduce our NS-NS and NS-BH merger models and their basic properties. Sec. 3 presents the r-process network and the nuclear models used as input and varied in this work. The results of our nucleosynthesis calculations and the impact of consistently propagating nuclear uncertainties into r-process calculations, including abundance distributions, heating rates and cosmocronometric age estimates are discussed in Sec. 4. In addition, a comparison to other works can be found in Sec. 4. A summary and conclusions are given in Sec. 5.

2 ASTROPHYSICAL MODELS

Our nucleosynthesis calculations are based on advanced computational models of the binary NS or NS-BH merger systems. However, fully consistent models, which include weak nucleonic reactions and cover all evolution phases over a wide range of binary parameters are not available at the present time. We have applied an approximate model for the total NS-NS (NS-BH) merger ejecta by combining three models for the dynamical ejecta from Ardevol-Pulpillo et al. (2019); Kullmann et al. (2021); Just et al. (2015a) with two BH-torus models from Just et al. (2015a).

The NS-NS merger simulations that produce the dynamical ejecta are based on a relativistic smoothed-particle-hydrodynamics (SPH) code coupled to the so-called improved leakage-equilibration-absorption scheme (ILEAS) for neutrino transport (Ardevol-Pulpillo et al. 2019). The ILEAS scheme goes beyond a conventional leakage scheme by accounting for re-absorption with a ray-tracing algorithm in the optically thin conditions, and adding an equilibration step in the optically thick regions in addition to an improved estimate of the neutrino diffusion timescales. ILEAS was designed to be more computationally efficient than the most sophisticated neutrino transport calculations in the literature, still it has been shown to satisfactorily reproduce local neutrino interaction rates in good agreement with state-of-the-art neutrino-transport solutions (Ardevol-Pulpillo et al. 2019).

To model the contribution from the NS-NS dynamical ejecta we have chosen two systems with a total mass of $M_1 + M_2 = 2.7 M_{\odot}$; one symmetric ($1.35 M_{\odot}$ - $1.35 M_{\odot}$) and one asymmetric ($1.25 M_{\odot}$ - 1.45$M_{\odot}$) merger with the SFHo...
EoS (Steiner et al. 2013), from now on referred to as model sfho-135-135 and sfho-125-145, respectively. For these systems, a delayed collapse of the HMNS remnant to a BH is expected to take place soon after the dynamical merger phase, i.e. some $\sim 10$ ms after the stars touch. Although the gravitational collapse did not yet occur at the end of the simulations at about $\sim 10$ ms after merging, we do not consider ejecta launched from the HMNS on time-scales longer than $\sim 10$ ms in this study. Although the amount of matter ejected during the HMNS evolution can in principle be comparable to the other ejecta components, the ejecta masses and other properties still carry large uncertainties, mainly because the magnetohydrodynamic effects responsible for angular momentum transport are yet poorly understood (see, e.g., Perego et al. (2014); Fujibayashi et al. (2018); Palenzuela et al. (2022); Shibata et al. (2021) for discussions of HMNS ejecta). In our cases, the HMNS phase will be relatively short, and thus neglecting the HMNS ejecta are an acceptable approximation and assumed to introduce uncertainties which are at the same level as the uncertainties presently existing in hydrodynamical simulations. The NS-BH binary system consists of a $1.1M_\odot$ NS and a $2.3M_\odot$ BH, also modelled with the SFHo EoS (referred to as sfho.1123 in Just et al. 2015a), from now on named sfho-11-23 (this model does not include neutrino effects which may be a decent approximation for the mostly tidally ejected material; ignoring neutrino emission and absorption may be a valid approximation because of the rapid expansion of mostly tidally ejected material in NS-BH mergers).

Given the challenge to obtain fully consistent models covering the entire merger evolution and the large uncertainties related to the viscosity of the disk models, we have chosen two BH-torus systems that approximately match the configurations obtained after the merger in models sfho-135-135, sfho-125-145, and sfho-11-23. For the post-merger phase we have used a BH mass of $3M_\odot$ and torus masses of 0.1 and $0.3M_\odot$, named as models M3a8m1a5 and M3a8m3a5-v2 in Just et al. (2015a). The BH-torus simulations are performed in Newtonian hydrodynamics with a modified gravitational potential (Artemova et al. 1996) to approximately model some relativistic effects like an innermost stable circular orbit. The neutrino transport is described by a truncated two-moment scheme (Just et al. 2015b) and to include the effects of turbulent angular momentum transport, two $\alpha$-viscosity approaches called “type 1” and “type 2” are applied in model M3a8m1a5 and M3a8m3a5-v2, respectively. See Just et al. (2015a) for a detailed discussion of the simulations and the adopted parameters.

Table 1 lists the hydrodynamical models and their properties including NS, BH or torus mass, spin and ejected mass. For the models covering the dynamical ejecta, the values refer to those extracted at the end of the simulation time ($t \sim 10$ ms after merging). In these simulations the merger remnant did not yet collapse to form a BH, and the torus mass is estimated by determining which fraction of matter is rotationally supported assuming a collapse took place (see Oechslin et al. (2007) for details). As can be seen in Table 1 the total outflow mass of the dynamical ejecta in the NS-NS models are 2-20 times less massive than the BH-torus ejecta, hence the total r-process abundance distribution is dominated by the BH-torus component. In contrast, in the NS-BH system the dynamical and secular ejecta masses are of the same order of magnitude.

The ejecta distributions of the electron fraction $Y_e$ and mass fraction of free neutrons $X_n^0$ at the network initiation time for the three merger models (a,b,c) and the two remnant models (c,d) are shown in Fig. 2, where the masses have been integrated over the simulated evolution time and normalised to the total ejected mass for each individual model. $X_n^0$ provides a better rough indicator of the efficiency of the r-process than the $Y_e$ alone (which is commonly used in the literature when discussing the conditions characterizing the r-process efficiency). By definition, a lower $Y_e$ gives a larger $X_n^0$, as can be seen in Fig. 2; however, a higher initial entropy will also give a larger $X_n^0$ due to the release of free neutrons through photodissociation (see for example Meyer 1989; Hoffman et al. 1997; Otsuki et al. 2000, for a discussion of the interplay between the $Y_e$, entropy, expansion time-scale and a successful r-process). For merger ejecta conditions with similar expansion timescales, it is only possible to produce the heaviest elements with a high $X_n^0$, while it is not always safe to conclude that heavy elements are only produced for $Y_e \lesssim 0.25$, because it is possible to have a successful r-process for $Y_e > 0.25$ if the entropy is sufficiently high. As can be seen in Fig. 2(e), the entire $X_n^0$ distribution lies above 0.8 for the NS-BH ejecta, which contrasts to the wide $X_n^0$ distribution obtained in the NS-NS simulations (Fig. 2(a,b)) that include neutrino interactions (see Kullmann et al. (2021) for a comparison to a “no-neutrino” case). Therefore, the NS-BH
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3 R-PROCESS CALCULATIONS AND NUCLEAR INPUT

The astrophysical simulations provide the detailed evolution of, among other variables, the temperature, density and entropy of the ejecta up to a few tens of ms or seconds, depending on the model. After that, the ejecta are assumed to expand freely at constant velocity so that the densities of the ejecta clumps decrease proportional to $1/t^3$. The r-process calculations are performed in a post-processing step starting from the initial composition given by the astrophysical environment and use the detailed evolution of the ejected mass elements (i.e. trajectories) to follow the expansion and abundance evolution up to $\sim 1$ year. We define the network initialization time to be the first time when both the temperature and density of a given trajectory drop below the threshold values of $T = 10 \times 10^9$ K and $\rho_{\text{dip}} \simeq 4.2 \times 10^{13}$ g cm$^{-3}$, respectively. Depending on the specific history of the trajectory followed and the astrophysical scenario modelled, the temperature may already be lower than 10 GK at the first time step, and in these cases the network calculation starts as soon as the density drops below the drip density $\rho_{\text{dip}}$. After the initialization time, the network includes the possible re-heating of the ejecta through $\beta$-decays, fission, and $\alpha$-decays so that the temperature evolution is calculated following the approach of Meyer (1989) using the laws of thermodynamics. The initial abundance of the heavy nuclei for each trajectory is determined by nuclear statistical equilibrium (NSE) at the given density $\rho_{\text{init}}$, temperature and electron fraction $Y_e$ at the initialization time. The nucleosynthesis is followed by a reaction network consisting of $\sim 5000$ species, ranging from protons up to $Z \simeq 110$ and including all isotopes from the valley of beta stability to the neutron drip line. For all these nuclei many nuclear ingredients and processes are required to calculate the abundance evolution. Our r-process reaction network includes all charged particle fusion reactions on light and medium mass isotopes, photodisintegrations, beta delayed neutron emission probabilities and the rates of radioactive neutron capture, $\beta$-decay and $\alpha$-decay. If the network reaches trans-Pb species we also include neutron induced, spontaneous and $\beta$-delayed fission and their corresponding fission fragment distributions for all fissile nuclei. Each fissioning parent is linked to the daughter nucleus and the emitted neutrons may be recaptured by the nuclei present in the environment. If a fission fragment is located outside the neutron drip line it is assumed to instantaneously emit neutrons to reach the neutron drip line.

Whenever experimental data is available it is included in the network. Reaction rates on light species are taken from the NETGEN library (Xu et al. 2013), which includes the latest compilations of experimentally determined rates. Since we lack experimental data for most of the $\beta$-unstable nuclei, in particular on the neutron-rich side, r-process network calculations rely on theoretical models which will be described in detail in the following sections.

Nuclear predictions are affected by systematic as well as statistical uncertainties. The former ones, also referred to as model uncertainties, are known to dominate for unstable nuclei (e.g., Goriely & Capote 2014) since there is usually no or very little experimental information available to constrain the model on those nuclei. Whenever experimental data are available, either for rates or reaction model ingredients, they are considered in the theoretical modelling. In this case, they also constrain the possible range of variation of the model parameters and reduce the impact on model as well as parameter uncertainties. However, for exotic nuclei, models of different natures, ranging between macroscopic to microscopic approaches (e.g., Arnould et al. 2007; Goriely 2015a; Hilaire et al. 2016; Plompen et al. 2017), may provide rather different predictions. For this reason, in the present study, global systematic uncertainties affecting reaction or decay rates will be considered. Those global systematic uncertainties are propagated to the calculation of reaction rates, and consistently applied to the nucleosynthesis simulations to estimate their impact on the r-process yields and decay heat.

The aim of this paper is to quantify the impact of the nuclear uncertainties on the r-process nucleosynthesis. We have performed r-process nucleosynthesis calculations on all available trajectories for each hydrodynamical simulation using a default set of the nuclear input. When adopting a variation of the default input we have calculated the nucleosynthesis abundances using a smaller subset of trajectories to reduce the computational demand. The subset of trajectories have been chosen in such a way that they contain a fraction of the total mass (see Table 1) while still representing the full data set in a satisfactory way, both for the abundance distribution

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1 Due to the large computational demand of varying the nuclear physics input for all hydrodynamical models, several of the calculations for the subset of NS-BH models were run with $Z = 100$ as the maximum limit for the network. The impact of this limitation has been tested and found to be negligible while significantly reducing the CPU time.

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Figure 2. (Color online) Fractional mass distributions of the matter ejected as a function of the mass fraction of free neutrons $X_n^0$ (left column) and electron fraction $Y_e$ (right column) at the network initiation time. The mean electron fraction $\langle Y_e \rangle$ and the mean initial neutron fraction $\langle X_n^0 \rangle$ are given for each merger and BH-torus models: a) shfo-125-145, b) shfo-135-135, c) M3A8m1a5, d) M3A8m3a5-v2 and e) shfo-11-23.
and the time evolution of the decay heat. In particular, the subset is chosen to ensure its $Y_e$ and $X^n_a$ mass distributions are similar to the one obtained with the full set of trajectories.

Table 2 lists the nuclear models considered for our uncertainty study, as described in the following sections. Unless otherwise specified, our calculations use input set 1 as default, and for $\alpha$-decay the model of Koura et al. (2002) has been used for all calculations. Note that all of the global models listed in Table 2 have proven their ability to describe experimental data with a high degree of accuracy (e.g., mass predictions should have an rms deviation below 0.8 MeV with respect to the 2400 experimentally known masses). Models that do not fulfill such a necessary requirement are not considered to be state-of-the-art and therefore excluded from our comparison study. However, accurately describing experimental data is a necessary but not a sufficient condition for a model to be applied to the $r$-process nucleosynthesis (for more details see Arnould et al. 2007). In summary, in order to best meet the nuclear-physics needs of the $r$-process, we require the applied models to be both accurate with respect to experimental observables, but also as reliable as possible, i.e., to be based on a physically sound model that is as close as possible to a microscopic description of the nuclear systems. This second criterion is fundamental for applications involving extrapolation away from experimentally known regions, in particular towards exotic neutron-rich nuclei of relevance for the $r$-process. Only nuclear physics models that fulfill the aforementioned criteria will be referred to in the following as “advisable” models. Not advisable are, for example, mass models like the Hartree-Fock-Bogolyubov (HFB) based on the SLy4 Skyrme interaction (Stoitsov et al. 2003) which poorly reproduces the full set of experimental masses with an rms deviation of 5 MeV in comparison with state-of-the-art mass models. Another example concerns some recent mass models based on machine learning algorithms (Shelley & Pastore 2021) which essentially consider mathematical rather than physical approaches and are consequently believed not to be suited for a reliable extrapolation far away from the experimentally known region.

### 3.1 Radiative neutron capture rates

Many nuclear structure properties are required to calculate the radiative neutron capture rates including mass model, nuclear level density, nuclear potential, $\gamma$-strength function, and for the non-resonant region even the energy, spin and parity of discrete states are needed. In the following discussion we will focus on to two different methods, namely the statistical Hauser-Feshbach method and the direct capture (DC) model for the estimation of radiative neutron capture rates.

**Compound nucleus and Direct capture**

The statistical Hauser-Feshbach reaction model is used as default in astrophysical applications to calculate the radiative neutron capture cross sections for experimentally unknown nuclei. Within the Hauser-Feshbach method the capture process is assumed to be a two-step process. First, a so-called compound nucleus (CN) is formed as an intermediate step. Second, the nucleus de-excites to the ground state of the residual nucleus by emitting a particle or a $\gamma$-ray. In this model the CN is assumed to be in thermodynamic equilibrium so that the energy of the incident particle is shared uniformly by all the nucleons before de-excitation. This assumption is expected to hold if we assume that the level density of the compound nucleus at the energy of the incident energy is large, and then the compound nucleus has an average statistical continuum superposition of available resonances at this energy. Although the Hauser-Feshbach method has proven to accurately reproduce cross sections for medium- and heavy-mass nuclei, the model suffers from uncertainties originating from the underlying theoretical nuclear models, and the validity of its CN assumption should be questioned for some light and neutron-rich nuclei for which only a few or no resonant states are available.

When the number of available states in the CN is relatively small, the neutron capture process may be dominated by the direct electromagnetic transition to a bound final state, without the formation of a compound nucleus. The direct capture (DC) process has been shown to be non-negligible compared to the Hauser-Feshbach component and can even contribute up to 100 times more to the total cross section for the most neutron-rich nuclei close to the neutron drip line (Sieja & Goriely 2021). The DC model also suffers from large model uncertainties mainly due to the remarkable sensitivity of the cross section to the few available final states, which for the very neutron-rich nuclei are unknown. The energy, spin and parity of the discrete levels can modify the DC contribution by many orders of magnitude since the selection rules which rely on the spin and parity differences may switch on or off the DC component (Xu & Goriely 2012).

It is normally assumed that the statistical and direct processes may contribute to the radiative neutron capture rate in a non-exclusive way. It remains, however, fundamental to...
use the same set of nuclear-structure ingredients to estimate both contributions. In particular, the same optical potential needs to be adopted to ensure the same total reaction cross section is found in both channels. According to the study of Xu et al. (2014), the experimental radiative neutron capture cross sections are in good agreement with the DC model for the lightest nuclei, where the CN model overestimates the contribution. For the experimentally unknown neutron-rich nuclei, the DC component contributes significantly to the total cross section, or even dominates over the CN contribution in some regions.

Both the DC and CN methods for calculating the theoretical radiative neutron capture rates are consistently included in the TALYS code (Goriely et al. 2008; Koning & Rochman 2012; Xu et al. 2014), which we use to estimate the rates. The reverse photoneutron emission rates, i.e. the $(\gamma,n)$ rates are calculated using detailed balance which includes an exponential dependence on the $Q$-value of the nuclei involved. Therefore, a large part of the sensitivity to the radiative neutron capture rates originates directly from uncertainties in the prediction of the neutron separation energy, hence of nuclear masses. Deviations in the mass predictions on the order of several MeV (see Sec. 3.2) translate into deviations in the neutron capture rates up to 3-5 orders of magnitude in certain regions of the nuclear chart. In Fig. 3 a comparison between the neutron capture rates obtained with the CN and CN plus DC component is displayed. We can see that the largest contribution from the DC component is for the neutron-rich nuclei and in certain regions in between the neutron magic numbers ($Z \sim 35 - 40$ and $Z \sim 50 - 70$). There are also large discrepancies in the fissile region ($Z > 90$), where the CN+DC component is over 100 times larger than the CN component. However, the impact of including the DC component in this region is not expected to be large, since the neutron-induced fission is expected to dominate over radiative neutron capture.

As default, all our r-process calculations are based on CN model rates, except for one variation of the nuclear inputs which also includes the DC component (see Table 2, input set 15). In this paper we have used the microscopic HFB plus combinatorial nuclear level densities (Goriely et al. 2008) and the E1 and M1 D1M+QRPA strength functions (with the inclusion of an empirical upbend) (Goriely et al. 2018). The cross section calculations are believed to be quite insensitive to varying the nuclear potential as long as they have the same volume integral per nucleon (Goriely 1997; Xu & Goriely 2012) and if the isovector imaginary potential remains large enough to ensure the neutron absorption (Goriely & Delaroche 2007). We will therefore use the same nuclear potential, the Woods-Saxon-type optical potential (KD; Koning & Delaroche 2003) for all calculations in this paper.

### 3.2 Nuclear mass models

The mass of the nucleus is one of the most crucial ingredients which many nuclear properties depend on. Although great

| Input set | Mass mod. | Direct capture | $\beta$ model | Fission barriers | Fission fragment |
|-----------|-----------|----------------|--------------|-----------------|-----------------|
| 1         | BSkG2     | no             | RHB+RQRPA    | HFB-14          | SPY             |
| 2         | FRDM12    | no             | RHB+RQRPA    | HFB-14          | SPY             |
| 3         | WS4       | no             | RHB+RQRPA    | HFB-14          | SPY             |
| 4         | D1M       | no             | RHB+RQRPA    | HFB-14          | SPY             |
| 5         | HFB-21    | no             | RHB+RQRPA    | HFB-14          | SPY             |
| 6         | HFB-31    | no             | RHB+RQRPA    | HFB-14          | SPY             |
| 7         | HFB-31    | no             | HFB21+GT2    | HFB-14          | SPY             |
| 8         | HFB-31    | no             | TDA          | HFB-14          | SPY             |
| 9         | HFB-31    | no             | FRDM+QRPA    | HFB-14          | SPY             |
| 10        | FRDM12    | no             | FRDM+QRPA    | HFB-14          | SPY             |
| 11        | FRDM12    | no             | TDA          | HFB-14          | SPY             |
| 12        | FRDM12    | no             | FRDM+QRPA    | HFB-14          | SPY             |
| 13        | HFB-21    | no             | RHB+RQRPA    | MS99            | GEF             |
| 14        | BSkG2     | no             | RHB+RQRPA    | MS99            | GEF             |
| 15        | HFB-21    | yes            | RHB+RQRPA    | HFB-14          | SPY             |
experimental progress has been made in the last decades to reach the exotic neutron-rich region and future large facilities, and the Facility for Rare Isotope Beams (Surman & Mumpower 2018), the Facility for Antiproton and Ion Research (FAIR) (Walker et al. 2013) and the Radioactive Isotope Beam Factory (RIBF) at RIKEN (Li et al. 2022) will certainly help to provide experimental masses deep inside the neutron-rich region, it will not be possible to measure the masses of the nuclei of most importance to the r-process in the years to come. Thus, our nucleosynthesis calculations will have to continue to rely on theoretical masses in the foreseeable future.

In order to compare mass models and measure their performance, it is common to calculate the square root mean square (rms) deviation between a given mass model and all of the ~ 2500 (Wang et al. 2021) experimentally measured masses. Ideally, a mass model should be able to provide not only the mass, but also the other nuclear properties like charge radii, quadrupole moments, fission barriers, shape isomers, as well as infinite nuclear matter properties. This way, it would be possible to evaluate the model’s performance not only based on its rms deviation from the known masses, but also according to other nuclear properties and constraints. The mass models considered here have rms deviations from about 0.3 to 0.8 MeV on all the 2457 \( Z, N \geq 8 \) known masses (Wang et al. 2021).

Many different approaches exist in order to calculate nuclear masses ranging from the first macroscopic classical models (e.g., liquid drop model) to microscopic models only relying on first principles (e.g., shell model). In between these two extremes there are many semi-empirical approaches where a theoretical description of the nucleus is combined with free parameters which are fitted to the known masses (and sometimes other nuclear properties). In the following, we will focus on global mass models that try to reproduce the masses of all nuclei lying between the proton and neutron drip lines, of relevance for astrophysical applications. For a review, see, e.g., Pearson (2001); Lunney et al. (2003).

**Microscopic-macroscopic approach**

The classical liquid drop model describes the nucleus as consisting of nucleons that behave like the particles in a drop of liquid. Based on this model, the semi-empirical mass formula (also known as the Bethe-Weizsäcker formula) (von Weizsäcker 1935) was developed and shown to be quite successful in reproducing the general trends observed in nuclear data. However, it fails to describe quantum effects and therefore several microscopic-macroscopic (Mic-Mac) models have been proposed where microscopic corrections are added to the liquid drop part to account for the quantum shell and pairing correlation effects. In this framework, the macroscopic and microscopic features are treated independently, both parts being connected exclusively by a parameter fit to experimental masses. The most sophisticated version of this macroscopic-microscopic mass formulas is the “finite-range droplet model” (FRDM) (Möller et al. 2016). The calculations are based on the finite-range droplet macroscopic model and the folded-Yukawa single-particle microscopic correction. The 31 independent mass-related parameters of the FRDM model are determined directly from a least-squares adjustment to the ground-state masses on all the masses available at that time. This fit leads to a final rms deviation of 0.61 MeV for the 2457 \( Z, N \geq 8 \) nuclei with experimental masses. Inspired by the Skyrme energy-density functional (see below), the so-called Weizsäcker-Skyrme (WS) macroscopic-microscopic mass formula was proposed by Wang et al. (2010, 2014); Liu et al. (2011) with an rms deviation of about 0.3 MeV. In such an approach, the mass formula is mathematically corrected by including a Fourier spectral analysis examining the deviations of nuclear mass predictions to the experimental data at the expense of a huge increase in the number of free parameters, and potentially a decrease in the predictive power of the model.

Despite the great empirical success of the macroscopic-microscopic approach, it suffers from major shortcomings, such as the incoherent link between the macroscopic part and the microscopic correction, the instability of the mass prediction to different parameter sets, or the instability of the shell correction (Pearson 2001; Lunney et al. 2003). The quality of the mass models available is traditionally estimated by the rms error obtained in the fit to experimental data and the associated number of free parameters. However, this overall accuracy does not imply a reliable extrapolation far away from the experimentally known region since models may achieve a small rms value by mathematically driven or unphysical corrections, or can have possible shortcomings linked to the physics theory underlying the model. As discussed above, the reliability of the mass extrapolation should be considered as a second criterion of first importance when dealing with specific applications such as astrophysics, but also more generally for the predictions of experimentally unknown ground and excited state properties. For this reason, microscopic mass models have been developed, as discussed below.

**Mean-field approach**

One of the most microscopic and successful model we have of the nucleus is the shell model, where the interaction between each individual nucleon (or each nucleon outside of a rigid core) is taken into account. However, due to the impossible task of solving the many-body problem for a large number of nucleons, e.g., due to the extreme computational demand, such a model can only be applied to light systems. Instead of calculating the interaction between all nucleons exactly, effective potentials describe the interaction of a nucleon with the mean field generated by all the other nucleons. By using microscopic nuclear many-body models as basis, relativistic or non-relativistic mean field approaches based on the density functional theory can calculate all the masses of the entire nuclear chart. However, fitting interaction parameters to essentially all mass data remains an extremely demanding task and, for this reason, most of these mean-field models have been adjusted on the properties of only a few nuclei. The underlying interactions of the microscopic models can also be used to calculate the EoS of infinite nuclear matter and neutron star material. This is an advantage for the mean-field models since it gives another application of the theoretical framework and provides additional model constraints as for example the maximum NS mass or mass-radius relations (e.g., see Fantina et al. 2013; Pearson et al. 2018). On the long run this approach may establish a consistency between the model of the network calculations and the EoS used in the astrophysical simulations, which is currently not considered.
In this work we consider mean-field mass models based on two different effective interactions, namely the Skyrme (Vautherin & Brink 1972) and finite-range Gogny (Gogny 1973) interactions. More specifically, we adopt the Gogny-D1M mass model (Goriely et al. 2009) which takes into account all the quadrupole correlations self-consistently and microscopically and reproduces the 2457 experimental masses (Wang et al. 2021) with an rms deviation of 0.81 MeV. Many versions of the Brussels-Montréal Skyrme-HFB mass models have been developed in a series of continuous improvements. We consider here the HFB-21 (Goriely et al. 2010) and HFB-31 (Goriely et al. 2016a) mass models with an rms deviation of 0.59 and 0.56 MeV, respectively, since both have been used previously in nucleosynthesis calculations. In addition, we also consider the BSkG2 mass model (Scamps et al. 2021) which is obtained through a three-dimensional coordinate-space representation of the single-particle wave functions allowing for both axial and triaxial deformations and treats nuclei with an odd number of nucleons in the same way as the even-even nuclei by breaking time-reversal symmetry. Its rms deviation amount to 0.68 MeV with respect to the 2457 known masses. Unless otherwise specified, we use BSkG2 as our default mass model.

In Fig. 4 the mass differences between BSkG2 and the other five mass models, as well as between both droplet-type parametrizations, are displayed. The mass difference can be over 6 MeV in some regions, where generally the largest deviations lie close to the driplines or in regions further from the neutron magic numbers for some models.

3.3 β-decay rates

β-decay rates remain crucial for the r-process nucleosynthesis since they define the time scale for the abundance flow to go from one Z to the next one. At later times, after freeze out, the β-decay and β-delayed neutron emission probabilities play an important role in determining the flow back to the valley of β-stability and also the energy release relevant for the kilonova light curve. Although β-delayed neutron emission occurs throughout the duration of the r-process, it is in particular important during the late phases when the competition between neutron captures and β-decays shapes the final r-process abundance distribution, in particular around the r-process peaks.

As with the other nuclear input properties required by the r-process, the experimental β-decay rates are included when available (Kondev et al. 2021), but for a large number of nuclei we have to apply theoretical rates from one of the few available global models. Similar to the mass models, microscopic shell model calculations for β-decay exist, but due to the computational cost they are restricted to nuclei near closed shells and cannot yet tackle the heavy, neutron rich nuclei required for r-process applications. One widely used model is gross theory, which allows for fast and reasonably accurate computation of the half-lives given the input of appropriate $Q_\beta$-values. The gross theory is based on β-decay one-particle strength functions to describe the general behaviour of β-decay. The one-particle strength functions and the pairing scheme has been improved in its GT2 version (Tachibana et al. 1990) based on the HFB-21 $Q_\beta$-values.

Several global semi-microscopic models are based on an effective interaction to describe the nuclear structure and adopt the random phase approximation (RPA), or its quasiparticle (QRPA) extension to include pairing interactions, to describe allowed Gamow-Teller decay. The FRDM+QRPA (Möller et al. 2003) model uses the FRDM $Q$-values and a separable residual interaction for the QRPA description of the Gamow-Teller transitions and also includes the gross theory for the first-forbidden transitions. One of the most reliable models available is the spherical relativistic Hartree-Bogoliubov (RHB) model plus relativistic QRPA (RQRPA) (Marketin et al. 2016) based on the DC3* residual interaction which also includes first-forbidden transitions.

Finally, the Tamm-Dancoff approximation (TDA) (Klappor et al. 1984) is another global model available that provides a simple analytical solution to calculate the β-decay strength distribution by using a simplified Gamow-Teller residual interaction, neglecting the influence of first-forbidden transitions on the half lives.

In Fig. 5 the ratio between the β-decay rates estimated by the relativistic mean field (RMF), i.e. RHB+RQRPA, and the HFB21+GT2, TDA and FRDM+QRPA as well as the ratio between the HFB21+GT2 and FRDM+QRPA predictions are shown. Major differences can be seen for exotic neutron-rich nuclei, in particular for $N > 126$, where, in particular, the RHB+RQRPA model is seen to predict larger rates. We apply all four β-decay models in Fig. 5 in our r-process calculations, where the RHB+RQRPA model is used as default (see Table 2). Note that when we change the applied mass model for our r-process calculations it directly impacts the estimated neutron capture rates, but not the β-decay rates since they are estimated separately by the models discussed above. Thus, due to the limited set of available global β-decay models, we often have an inconsistency between the mass model applied in the r-process calculations and the masses used to calculate the $Q_\beta$-values. Therefore, a future prospective is to develop fully consistent models for all nuclear physics input applied in r-process calculations.

3.4 Fission models for r-process applications

In sufficiently neutron-rich astrophysical scenarios ($X_n^0$ typically larger than 0.7), the r-process can reach nuclei in the $Z \geq 90$ region where fission may become the dominant mode of decay. It is often said that fission terminates the r-process because it stops the abundances from reaching even further up in the super-heavy region of the nuclear chart, and recycles material back to the 100 $\lesssim A \lesssim 180$ region. Given sufficient time before freeze-out, these daughter nuclei may again be involved in a series of neutron captures and β-decays before reaching the fissile region for the second time. This is often referred to as “fission recycling”. In addition to producing daughter nuclei, fission also contributes to the r-process by releasing neutrons that may be recaptured by the network. This late neutron production can give the neutron capture phase a boost and impact the final abundance distribution after freeze-out. Another important aspect of fission during the r-process is that it releases heat which can impact the kilonova light curve. In particular the spontaneous fission of $^{254}$Cf with a half life of 60 days has been shown to be important for the energy generation and to impact the light curve at $t > 100$ days (Wanajo 2018; Wu et al. 2019; Zhu et al. 2018).

Fission is a very complex nuclear process and a variety of
Figure 4. (Color online) Similar to Fig. 3 for mass difference $\Delta m$ between different mass models listed in Table 2. Mass differences larger or smaller than the maximum or minimum values of the color bar ($\pm 6$ MeV) are represented by red and blue, respectively.

Figure 5. (Color online) Similar to Fig. 3 where the ratio between the $\beta$-decay rates predicted by the four models listed in Table 2 are plotted in the $(N,Z)$ plane. Differences larger or smaller than the maximum or minimum values of the colour bar ($10^{\pm 1.5}$ MeV) are represented by blue and red, respectively.
nuclear structure inputs are required to achieve a successful model. For the r-process, we need models describing the probability for a nucleus to undergo neutron-induced, spontaneous and β-delayed fission, but also fission fragment distributions to determine the daughter nuclei and the number of free neutrons released. Photo-induced fission is assumed to be unimportant since the temperatures have typically fallen below 1 GK by the time the r-process network reaches the fissile region. In this work we have used either the HFB-14 fission paths based on the BSk14 Skyrme interaction² (Goriely et al. 2010) or the Thomas-Fermi model (Myers & Świątecki 1999, hereafter MS99) to estimate the fission rates. Fig. 6 shows the regions where fission processes dominate over other decay modes or neutron capture for the HFB-14 and MS99 fission barriers using either mass model HFB-21 or BSkG2 for the calculation of the neutron capture rates. The MS99 barriers are usually lower than the predictions of the HFB model so that more nuclei are found to be affected by fission processes when the MS99 barriers are adopted. Note that the MS99 barriers are not always available for very exotic n-rich nuclei close to the neutron-drip line, especially for $Z > 106$. In these cases, the HFB-14 barriers are adopted. During the freeze-out phase, if we adopt the HFB-14 fission barriers, fission takes place around $Z \approx 101 \pm 102$ along the abundant $A \approx 278$ isobar, while the lower MS99 barriers lead to fission already around the $Z \approx 95 \pm 97$ isotopes. The applied mass model impacts the balance between neutron-induced fission and neutron capture through the calculation of the neutron capture rates, but also through the position of the neutron drip line since this determines which nuclei are available to fission. This is illustrated in Fig. 6 where we can see that mass model HFB-21 allows for fission in a large region for $N > 230$, while mass model BSkG2 predicts this region to be unstable for neutron emission.

For the fission fragment distributions we adopt either the renewed microscopic Scission Point Yield (SPY) model (Lemaître et al. 2019, 2021) or the 2018 version of the semi-empirical GEF model (“Général description of Fission observables”) (Schmidt et al. 2016). Unless otherwise specified, we use the HFB-14 barriers and the SPY fission fragment distributions as default for our calculations.

4 IMPACT ON THE R-PROCESS NUCLEOSYNTHESIS

In the following section the nucleosynthesis results obtained when varying the nuclear input discussed in Sect. 3 will be presented. First we show the r-process nucleosynthesis distributions and heating rates obtained using the astrophysical models for the dynamical and BH-torus ejecta separately, before we discuss the results for the combined ejecta and the cosmochronometric age estimates for six r-process enhanced metal-poor stars. For each nuclear input set, all quantities (except those presented in Fig. 22) are mass averaged over

² Ideally, the fission paths should be calculated based on the same interaction as the mass models applied in the r-process calculations (i.e. HFB-21 and so on, see Table 2). However, fission barrier calculations are very expensive, and therefore only a few global models suitable for astrophysical applications are available.
tical models sfho-125-145 and sfho-135-135. The largest differences between both sets of rates are found around $A \sim 150$ where the model including the DC component has a peak structure (double lanthanide peak), and in particular for model sfho-125-145 the third r-process peak is also wider when the DC is included.

The heating rate is defined here as the radioactive energy release rate per unit of mass due to $\beta$-decay, $\alpha$-decay, and fission:

$$Q = Q_\beta + Q_\alpha + Q_{\text{fiss}},$$

not including the contribution lost into neutrino emission $Q_\nu$, and globally follow the approximated trend given by

$$Q_0 = 10^{10}[t/1 \text{ day}]^{-1.3}\text{erg/g/s}.$$ (4)

The effective heating rate $Q_{\text{heat}}$ measures the fraction of radioactive energy that is converted into thermal energy in the expanding ejecta, i.e. the energy that actually powers the kilonova, defined as:

$$Q_{\text{heat}} = Q_{\text{therm}} \cdot (Q + Q_\nu),$$ (5)

where the total thermalization efficiency $f_{\text{therm}}$ is calculated as in Just et al. (2021a) (which is based on Rosswog et al. (2017) and Barnes et al. (2016)).

Fig. 11(a-b) shows the time evolution of the heating rate $(Q)$ for all combinations of nuclear models (see Table 2) for the dynamical ejecta of the NS-NS systems. All nuclear models predict about the same r-process heating, except for the peak around $t \sim 0.2$ hours, where the calculations using the FRDM12 mass model (see Fig. 9) show extra heating due to the energy generated by $\beta$-decay. This enhancement is mostly related to the larger $A = 88$ abundance predicted by the calculations that apply the FRDM12 mass model (input sets 2 and 10-12 in Table 2) and the $\beta$-decay of $^{88}\text{Kr}$ to $^{88}\text{Rb}$ and $^{88}\text{Rb}$ to $^{88}\text{Sr}$. After $t > 30$ days the contribution to the heating rate from fission differs between the nuclear input cases, where the largest heating is found when using mass model FRDM12 and either FRDM+QRPA, HFB21+GT2 or TDA $\beta$-decay rates.

4.1.2 NS-BH merger

Fig. 7c displays the composition estimated when varying the six mass models for the NS-BH merger model sfho-11-23. We can see that compared to the dynamical ejecta of the NS-NS merger systems (panels a and b), the NS-BH merger ejecta undergoes a strong r-process and follows the solar system r-process distribution for $A \gtrsim 140$ (compared to $A \gtrsim 90$ for NS-NS systems). The astrophysical conditions lead to a weak second r-process peak, and an additional structure around $A \sim 140$ due to fission processes (see below); however the strength of this structure varies between the mass models and is found to be particularly strong for mass model HFB-31.

When varying the models for the $\beta$-decay rates in Fig. 8c (using mass model HFB-31), the structure around $A \sim 140$ is present with the same strength, which was not always the case for the NS-NS merger models. However, large deviations are found for $A > 160$ in Fig. 9c, which shows the impact of the $\beta$-decay models when using mass model FRDM12.

The material ejected from the NS-BH merger model has initial conditions that favour a larger production of fission material in comparison with the NS-NS merger models considered here and are therefore well suited to study the impact of varying the fission properties. In Fig. 11c we can see that the impact of fission on the heating rate at $t > 30d$ is larger compared to the NS-NS merger models.

In Fig. 12 we see that fission barriers and fragment distributions significantly affect the predicted abundance distributions (and proportionally more than varying the mass model). All models predict about the same amount of actinides (2-2.5%), however MS99+GEF predicts a sharper peak at $A \sim 165$ than HFB-14+SPY. The asymmetric nature of the fission fragment distribution, in particular around $A \sim 278$ isobars is also found to impact the final abundance distribution in the $A \gtrsim 140$ region, as already pointed out by Goriely et al. (2013).

4.2 BH-torus ejecta

The material which is ejected in the post-merger phase from the torus surrounding the BH has quite different conditions than the dynamical ejecta (see Fig. 2), and therefore the r-process distribution differs in its shape, as seen in Figs. 13–15 for the various mass and $\beta$-decay models. In general, the disk wind models produce more nuclei in the $A \sim 80$ region, and in particular model M3Anna8m3a5-v2 produces less of 3rd peak elements and actinides, which is also where the largest differences between the mass models can be seen. The shape of the
Nuclear uncertainties and $r$-process in NS mergers

Figure 8. (Color online) Same as Fig. 7 when varying the four models for the $\beta$-decay rates, but using the same HFB-31 mass model (i.e. input sets 6-9 in Table 2). See the text for references and details about the different models. The solar system abundance distribution is normalized as in Fig. 7.

Figure 9. (Color online) Same as Fig. 7 when varying the four models for the $\beta$-decay rates, but using the same FRDM12 mass model (i.e. input sets 2 and 10-12 in Table 2). See the text for references and details about the different models. The solar system abundance distribution is normalized as in Fig. 7.

Figure 10. (Color online) Same as Fig. 7 when including the DC component for the radiative neutron capture rates, but using the same mass model, the HFB-31 model (i.e. input sets 5 and 15 in Table 2). See the text for references and details about the different models. The solar system abundance distribution is normalized as in Fig. 7.

peak around $A \sim 132$ also differs, where a very narrow structure can be seen for the M3A8m3a5-v2 model\(^3\), compared to the wider peak for model M3A8m1a5 and the dynamical ejecta.

Figs. 14-15 show the $r$-process results when varying the four models for the $\beta$-decay rates and the two mass models HFB-31 and FRDM12, respectively. Just as for the dynamical ejecta, the HFB-31 mass model combined with the TDA or GT2 $\beta$-decay models overproduce abundances for nuclei around $A \sim 130 - 140$.

The time evolution of the heating rate is shown in Fig. 17 for all the 15 nuclear models. We can see that the heating rate varies less for different nuclear models in the BH-torus ejecta than in the dynamical ejecta (Fig. 11). The nuclear mass models only start to differ significantly at $t > 10$ d for model M3A8m1a5 due to the larger production of heavy and fissile $r$-process elements. Model M3A8m3a5-v2 displays a peak at around 0.2 and 10 d due to the $\beta$-decays of $A \sim 88$ and $\sim 140$ nuclei, respectively, and has a negligible contribution from fission and $\alpha$-decay at late time ($t > 20$ d).

4.3 Combining dynamical and BH-torus ejecta

The sensitivity to the nuclear physics input when we combine the material from the dynamical ejecta with the post-merger BH-torus ejecta are displayed in Figs. 18, 19, 20 and 21. Since

\(^3\) This feature is also observed in Wu et al. (2016) and is related to trajectories, in which material falls back towards the torus and gets re-heated before it ultimately becomes ejected.

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Figure 11. (Color online) Time evolution of the radioactive heating rate $Q$ (before thermalization) for our NS–NS and NS–BH dynamical ejecta merger models: a) sfho-135-135, b) sfho-125-145 and c) sfho-11-23 when varying the nuclear input between all models listed in Table 2. The gray dashed line corresponds to the approximation $Q_0 = 10^{10}[t/1 \text{day}]^{-1.3}$ erg/g/s. The ratio $Q/Q_0$ is also shown as an insert, where the line $y=1$ is indicated by the gray dashed line. See Figs. 7, 8, 9 and 10 for the color labels for each nuclear input combination.

Figure 12. (Color online) Same as Fig. 7c when varying the fission barriers and fragment distributions, using the mass model HFB-31 or BSkG2 (i.e. input sets 1, 5, 13 and 14 in Table 2) for the material ejected by our NS–BH merger model sfho-11-23. See the text for references and details about the different nuclear models. The solar system abundance distribution is normalized as in Fig. 7c.

Figure 13. (Color online) Final mass fractions of the material ejected as a function of the atomic mass $A$ for our two BH-torus models (M3A8m1a5 and M3A8m3a5-v2) when varying between six mass models (i.e. input sets 1-6 in Table 2). See the text for references and details about the different models. The solar system r-abundance distribution (open circles) from Goriely (1999) is shown for comparison and arbitrarily normalized at the third r-process peak of model M3A8m1a5.

Figure 14. (Color online) Same as Fig. 13 when varying the models for the $\beta$-decay rates, but using the same HFB-31 mass model (i.e. input sets 6-9 in Table 2). See the text for references and details about the different models. The solar system abundance distribution is normalized as in Fig. 13.

The radioactive heat generated from the separate decay modes $Q_\beta$, $Q_\alpha$ and $Q_{\text{fus}}$ and the total heating rate $Q$ are so that in this case the total ejecta given in Fig. 18h show a composition where both components play a significant role and that is found to resemble the solar system distribution fairly well for $A > 90$.
of heavy r-process elements produced and the detailed decay path taken back to the stable or long-lived nuclei, while it is not affected by the involved α-decay rates since these are experimentally known. Model sfho-125-145 plus M3A8m3a5-v2 generates fewer trans-Pb species than models sfho-135-135 plus M3A8m1a5 and sfho-11-23 plus M3A8m3a5-v2, and therefore $Q_\alpha$ has an insignificant impact on the total heating rate for this model. All of the nuclear input sets generate heat from the α-decay chain starting from $^{224}$Ra, however, only a few input sets have non-negligible contributions from other decay chains. In particular, for input sets 9, 10, 12 and 13 that apply the TDA or FRDM+QRPA β-decay models (see Table 2), the heat generated by the α-decay chains starting from $^{223}$Ra, $^{225}$Ac or $^{221}$Fr leads to a large increase in $Q_\alpha$. This is related to the faster β-decay rates for the most neutron deficient $Z > 83$ nuclei (see Fig. 5) for models TDA and FRDM+QRPA, but also to the larger production of heavy r-process elements for these models.

The $Q_{fis}$ curve is completely dominated by the spontaneous fission of $^{254}$Cf, no other fissile nuclei generate any considerable heat. Therefore, the impact on $Q_{fis}$ arising when varying the nuclear physics input is related to the ability of a particular input set to produce the heaviest elements, which is not only sensitive to the various fission models, but all of the nuclear physics properties considered in this work.

As discussed earlier, the differences for $Q_\beta$ at $t \sim 0.2$ d 4} See the supplemental material of Wu et al. (2019) for a complete list of the most important α-decay chains contributing to the heating rate and also the discussion in Kullmann et al. (2021) for the dynamical ejecta models applied in this work.
are mostly due to the larger production of $A = 88$ nuclei for the FRDM12 mass model (see Figs. 11 and 17), but also nuclei in the $A \sim 130$ region. Later, at $t \sim 10$ d, another enhancement can be seen in the heating rate which is in particular strong for the combined ejecta models involving the BH-torus model M3A8m3a5-v2 (i.e. the two bottom panels of Fig. 20). This structure in the heating rate is related to the $\beta$-decay of $^{132}$I, which forms the over-abundance peak at $A = 132$ seen in Fig. 13, as discussed earlier.  

Fig. 21 shows the effective heating rate $Q_{\text{heat}}$ as well as the total thermalization efficiency $f_{\text{therm}}$. Note that $f_{\text{therm}}$ already starts well below 1 due to the energy lost to neutrinos (contained in $Q_{\nu}$). For the astrophysical models studied here, we can see that the biggest impact on the thermalization efficiency comes when varying the $\beta$-decay rates and fission properties. More specifically, a significant enhancement is found when adopting the FRDM+QRPA, TDA or HFB21+GT2 models (input sets 7-12) compared to the RHB+RQRPA rates, in particular for model sfho-135-135+M3A8m1a5.  

As discussed above, varying the $\beta$-decay model leads to variations in $Q_{\nu}$ and $Q_{\text{th}}$ (see Fig. 20) which in turn contribute to the $f_{\text{therm}}$ variations seen for $t > 10$ d in Fig. 21. Varying the fission properties also impacts the thermalization efficiency, however to a lesser extent than varying the $\beta$-decay model. The masses have a secondary impact on the thermalization efficiency, though results with FRDM (input set 2) and WS4 (input set 3) mass models deviate significantly from the other models (input sets 1, 4-6).

For convenience, Table 3 summarizes several $r$-process process including the mass fraction of strontium, lanthanides plus actinides ($X_{\text{LA}}$), $A > 69$ and $A > 183$ nuclei together with the heating rate at 1 d for all models studied in this work.

### 4.4 Impact on cosmochronometers

Based on the sensitivity analysis performed above, we can estimate the impact of the nuclear uncertainties on the production of the Th and U cosmochronometers and estimate the age of specific metal-poor stars for which the surface abundances of Th and U have been determined. In Table 4 the mean estimated ages for six metal-poor stars are listed assuming they have been initially polluted by the combined ejecta corresponding to our models for the NS-NS or NS-BH merger. The age is calculated by using eq. 2 with the $r$-process abundance ratio of $(\text{Th}/U)$, consistently obtained from our three combined ejecta models and the 15 different nuclear inputs and the observed abundance ratios $(\text{Th}/U)_{\text{obs}}$ from the literature (see Table 4 for the references). In addition, the standard deviation from the mean arising when varying the nuclear physics input is listed for the $(\text{Th}/U)_r$ ratio and stellar ages. The average ages obtained for all different nuclear physics inputs vary from 11.2 to 18.8 Gyr depending on the star and astrophysical model applied. The theoretical Th/U ratio for combined models sfho-135-135+M3A8m1a5 and sfho-11-23+M3A8m3a5-v2 is similar, leading to almost identical age estimates, while model sfho-125-145+M3A8m3a5-v2 has a larger Th/U ratio giving in general smaller age estimates. It is also model sfho-125-145+M3A8m3a5-v2 that has the largest spread in the calculated values when varying the nuclear physics inputs. For example, the age of star CS22892-052 ranges between 7.9 and 14.4 Gyr for the maximum and minimum ages, respectively. It is always input set 7 (which applies mass model HFB-31 and $\beta$-decay model HFB21+GT2, see Table 2) that gives rise to the minimum age estimate. The maximum age is found with input sets 5, 4 and 15 (using mass models HFB-21 or D1M) for models sfho-135-135+M3A8m1a5, sfho-125-145+M3A8m3a5-v2 and sfho-11-23+M3A8m3a5-v2, respectively. The observational uncertainties for the Th/U ratios and the age estimates ($\sigma_{\text{obs}}$) are also listed in Table 4. We calculate the observational uncertainty of the Th/U ratios as the square root of the quadratic sum of the Th and U abundance uncertainties provided by the references listed in Table 4 and propagate the observational uncertainty of the ratios to the age estimate ($\sigma_{\text{obs}}$). We can see that the observational uncertainties are in general significantly larger than the uncertainties stemming from the nuclear physics input ($\sigma_s$).

### 4.5 Comparison with other works

Many r-process studies in the last decade have focused on the impact of the nuclear physics uncertainties on the r-process yields (Caballero et al. 2014; Mendoza-Temis et al. 2015; Eichler et al. 2015; Goriely 2015b; Martin et al. 2016; Lidick, et al. 2016; Mumpower et al. 2016; Nishimura et al. 2016; Bliss et al. 2017; Denissenkov et al. 2018; Barnes et al. 2021; Vassh et al. 2019; Nikas et al. 2020; Sprouse et al. 2020; McKay et al. 2019; Giuliani et al. 2020; Zhu et al. 2021; Barnes et al. 2021). Often, the goals of such studies are to identify specific nuclei, or regions in the nuclear chart where the r-process has the largest sensitivity to the experimentally unknown nuclear properties. If such nuclei are identified, they can be targeted by experimental campaigns, as long as they are within the reach of the given facility (e.g., Surman & Mumpower 2018). Another aim for r-process sensitivity studies is to estimate the magnitude of the nuclear uncertainties so that they can be compared to other sources of uncertainty like those arising from the hydrodynamical modelling. This is in particular important for applications like cosmochronometry, galactic chemical evolution or kilonova models, which require r-process yields from a given site or ejecta component as input. A large range of astrophysical conditions has been applied in various r-process sensitivity studies in the literature, making detailed comparisons between results difficult. In the following we will, in a quantitative way, compare our results to other sensitivity studies that apply the same or similar nuclear models and ejecta components as we do and as summarised in Table 5.

Since the r-process is very sensitive to the conditions of the environment, it is important to keep in mind which assumptions and simplifications have been applied for the nucleosynthesis calculations. Basically three approaches of modelling the r-process conditions exist for a given astrophysical site or ejecta component: 1) parametrized trajectories which typically only depend on the initial electron fraction, entropy and expansion time scale, or 2) a single or a few (< 10) trajectories extracted from an hydrodynamical simulation, or 3) the full set (or a significant sample) of trajectories representing all the mass elements ejected, as given by an hydrodynamical simulation. Although the first two methods are simple idealisations, their obvious benefit is that the required computing time is significantly smaller than for the...
Table 3. The strontium mass fraction $X_{\text{Sr}}$, lanthanide plus actinide mass fraction $X_{\text{LA}}$, the mass fractions of r-process nuclei ($A > 69$) and third-r-process peak nuclei ($A > 183$), and the radioactive heating rate before thermalization $Q(t = 1 \text{d})$ at 1 day for the three dynamical, two BH-torus and the two combined ejecta models considered in the present study. For each quantity, the minimum (min), maximum (max), mean and standard deviation from the mean ($\sigma$) arising from the variation of the nuclear physics input sets in Table 2 are shown.

|         | $X_{\text{Sr}}$ | $X_{\text{LA}}$ | $X_{A>69}$ | $X_{A>183}$ | $Q(t = 1\text{d})\ [10^{10} \text{ erg/g/s}]$ |
|---------|----------------|----------------|--------------|--------------|------------------------------------------|
| sfho-125-145 | min 0.01 | 0.10 | 0.95 | 0.11 | 0.99 |
|         | max 0.09 | 0.15 | 0.97 | 0.18 | 1.20 |
|         | mean 0.04 | 0.12 | 0.97 | 0.15 | 1.10 |
|         | $\sigma$ 0.029 | 0.016 | 0.005 | 0.024 | 0.050 |
| sfho-135-135 | min 0.03 | 0.09 | 0.93 | 0.10 | 1.00 |
|         | max 0.11 | 0.15 | 0.95 | 0.19 | 1.20 |
|         | mean 0.06 | 0.11 | 0.95 | 0.15 | 1.09 |
|         | $\sigma$ 0.032 | 0.014 | 0.006 | 0.027 | 0.047 |
| sfho-1123 | min $4 \cdot 10^{-5}$ | 0.21 | 0.99 | 0.19 | 0.78 |
|         | max $4 \cdot 10^{-4}$ | 0.38 | 1.00 | 0.52 | 1.15 |
|         | mean $10^{-4}$ | 0.30 | 1.00 | 0.43 | 0.91 |
|         | $\sigma$ $10^{-4}$ | 0.056 | 0.002 | 0.100 | 0.111 |
| M3A8m3a5-v2 | min 0.01 | 0.06 | 0.93 | 0.01 | 1.15 |
|         | max 0.07 | 0.10 | 0.96 | 0.13 | 1.41 |
|         | mean 0.04 | 0.08 | 0.95 | 0.05 | 1.32 |
|         | $\sigma$ 0.015 | 0.012 | 0.007 | 0.031 | 0.083 |
| M3A8m1a5 | min 0.02 | 0.06 | 0.94 | 0.09 | 1.15 |
|         | max 0.03 | 0.11 | 0.95 | 0.15 | 1.47 |
|         | mean 0.02 | 0.08 | 0.94 | 0.12 | 1.31 |
|         | $\sigma$ 0.005 | 0.014 | 0.003 | 0.020 | 0.081 |
| sfho-125-145 + M3A8m3a5-v2 | min 0.02 | 0.07 | 0.93 | 0.02 | 1.18 |
|         | max 0.07 | 0.11 | 0.95 | 0.06 | 1.38 |
|         | mean 0.04 | 0.09 | 0.95 | 0.05 | 1.31 |
|         | $\sigma$ 0.015 | 0.013 | 0.005 | 0.009 | 0.061 |
| sfho-135-135 + M3A8m1a5 | min 0.02 | 0.07 | 0.94 | 0.09 | 1.14 |
|         | max 0.04 | 0.12 | 0.95 | 0.15 | 1.43 |
|         | mean 0.03 | 0.08 | 0.94 | 0.12 | 1.29 |
|         | $\sigma$ 0.007 | 0.014 | 0.003 | 0.020 | 0.075 |
| sfho-1123 + M3A8m3a5-v2 | min 0.01 | 0.12 | 0.95 | 0.09 | 1.06 |
|         | max 0.05 | 0.20 | 0.98 | 0.27 | 1.31 |
|         | mean 0.02 | 0.16 | 0.96 | 0.19 | 1.17 |
|         | $\sigma$ 0.010 | 0.025 | 0.005 | 0.047 | 0.065 |

Table 4. Age estimates of 6 metal-poor r-process enhanced stars based on the Th/U cosmochronometry (see eq. 2). The observational ratios, $(\text{Th/U})_{\text{obs}}$, and their corresponding uncertainty are from the references listed, and the $(\text{Th/U})_{r}$ ratios are taken directly from our r-process calculations using our three astrophysical models for the combined ejecta. The minimum, maximum and mean of the Th/U ratio as well as the standard deviation from the mean ($\sigma_{\log(\text{Th/U})}$) and the stellar age ($\sigma_{t^*}$) arising from varying the nuclear input sets listed in Table 2 are given for the three astrophysical models. Note that $\sigma_{t^*}$ is identical for all stars within each hydrodynamical model since a change in the observed Th/U ratio only leads to a shift in the estimated age. If the uncertainty of log(Th/U)_{obs} is not provided by the references, we calculate it as the square root of the quadratic sum of the individual, observational Th and U uncertainties given, and propagate it to the age estimates ($\sigma_{t^*\text{obs}}$).

| log(Th/U)$_{\text{obs}}$ | $\sigma_{t^*\text{obs}}$ | ref. | sfho-135-135 + M3A8m1a5 | sfho-125-145 + M3A8m3a5-v2 | sfho-1123 + M3A8m3a5-v2 |
|-------------------------|------------------|-----|---------------------|---------------------|---------------------|
| log(Th/U)$_{r,\text{min}}$ | - | - | 0.04 | 0.07 | 0.08 |
| log(Th/U)$_{r,\text{max}}$ | - | - | 0.31 | 0.37 | 0.34 |
| log(Th/U)$_{r,\text{mean}}$ | - | - | 0.18 | 0.21 | 0.18 |
| $\sigma_{\log(\text{Th/U})}$ | - | - | 0.10 | 0.10 | 0.08 |
| $\sigma_{t^*}$ | - | - | 1.9 Gyr | 2.1 Gyr | 1.7 Gyr |
| CS22892-052 | 0.73 ±0.22 | 4.9 Gyr | Sneden et al. (2003) | 12.0 Gyr | 11.2 Gyr | 12.1 Gyr |
| CS29497-004 | 1.04 ±0.33 | 7.2 Gyr | Hill, V. et al. (2017) | 18.8 Gyr | 18.0 Gyr | 18.8 Gyr |
| CS31082-001 | 0.94 ±0.21 | 4.7 Gyr | Siqueira Mello et al. (2013) | 16.6 Gyr | 15.8 Gyr | 16.6 Gyr |
| HE1523-0901 | 0.86 ±0.13 | 2.8 Gyr | Frebel et al. (2007) | 14.8 Gyr | 14.1 Gyr | 14.9 Gyr |
| J0954+5246 | 0.82 ±0.22 | 4.9 Gyr | Holmbeck et al. (2018) | 14.0 Gyr | 13.2 Gyr | 14.0 Gyr |
| J2038-0023 | 0.90 ±0.20 | 4.4 Gyr | Placco et al. (2017) | 15.7 Gyr | 14.9 Gyr | 15.8 Gyr |
Figure 18. (Color online) Final mass fractions of the material ejected as a function of the atomic mass $A$ when varying all nuclear models listed in Table 2 for each hydrodynamical model: a) sfho-135-135, b) sfho-125-145, c) sfho-11-23, d) M3A8m1a5 and e) M3A8m3a5-v2. The total ejecta (bottom panels) are calculated by summing the dynamical ejecta (top panels) with the BH-torus ejecta (middle panels), weighted by their respective ejected masses. For example panel f) is calculated as $X_f = (X_aM_a + X_dM_d)/(M_a + M_d)$, and similarly panel g) by combining b) and e), and h) by combining c) and e). The color scheme for the nuclear models are consistent throughout the article. The solar system r-abundance distribution (open circles) from Goriely (1999) is shown for comparison and arbitrarily normalized to the combined ejecta models (i.e. panel a, d use the normalisation from f, panel b from g, and panel c and e from h).

Figure 19. (Color online) Same as Fig. 18 panel f), g) and h) for the combined ejecta models zoomed in on the third r-process peak.
Figure 20. (Color online) Time evolution of the radioactive heating rate $Q$ (before thermalization) for the combined dynamical and secular ejecta for model sfho-135-135 plus M3A8m1a5 (top), sfho-125-145 plus M3A8m3a5-v2 (middle) and sfho-11-23 plus M3A8m3a5-v2 (bottom) when varying the nuclear input between all models listed in Table 2. The columns display the heating generated by $\beta$-decay ($Q_{\beta}$), $\alpha$-decay ($Q_{\alpha}$), fission ($Q_{\text{fis}}$) and the total heat from all or the decay modes ($Q = Q_{\beta} + Q_{\alpha} + Q_{\text{fis}}$). The gray dashed line corresponds to the approximation $Q_0 = 10^{10}[t/1 \text{ day}]^{-1.3} \text{ erg/g/s}$ The ratio $Q/Q_0$ is also shown as an insert in the right column, where the line $y = 1$ is indicated by the gray dashed line. See Figs. 13, 14, 15 and 16 for the color labels for each nuclear input combination.

son of Figs. 22 and 18 shows that uncertainty studies based on a single or a few trajectories may artificially exacerbate the impact of nuclear physics uncertainties, particularly in cases of $Y_e \sim 0.2 - 0.3$ close to the threshold of lanthanide production. One should consequently be careful when drawing conclusions regarding the total r-process yields of a given site or ejecta component from single-trajectory studies.

Another critical point in the comparison of sensitivity analyses concerns the way nuclear uncertainties are propagated to the nucleosynthesis calculations. A popular technique used to propagate the nuclear uncertainties to the final r-process results is to increase or decrease, for example, the nuclear mass or the neutron capture rate of a single nucleus by a given factor (e.g., see Surman & Mumpower 2018; Bliss et al. 2017, who applied factors of 5, 10, 50 or 100 to the $\text{(n,}\gamma\text{)}$ or $(\alpha,\text{n})$ rates). Then, for each variation or change of, for example, the nuclear mass of a given nucleus, the r-process abundances are re-calculated and compared to a base calculation with fixed nuclear (and astrophysical) input. After multiple variations, i.e. r-process calculations, the nuclei for which the abundances are the most sensitive with respect to changes of a given nuclear property are revealed. This technique can be seen as a variant of the MC method (see Mumpower et al. 2016; Rauscher 2020, for details about various implementations) since it applies random variations of quantities, such as mass, $\beta$-decay half lives, neutron capture rates or $\beta$-delayed neutron emission, pulled from a distribution which represents the assumed nuclear uncertainty of the property investigated. When considering uncertainties arising from (theoretical) nuclear physics inputs like for example the nuclear mass or neutron capture rates, there are two sources of uncertainty, namely statistical and systematic errors, where the latter is often referred to as model errors. MC studies adopt a given nuclear model for the baseline calculation (i.e. they have to choose the mean of the uncertainty distribution) and consider uncorrelated variations around that baseline. Therefore MC methods and similar techniques can, by design, only probe uncorrelated statistical errors. The claim that the independent and random variations of the nuclear properties of individual nuclei can probe all nuclear uncertainties, including the systematic model uncertainties (Mumpower et al. 2016, and references therein) would only be correct if the nuclear properties addressed by the MC studies were uncorrelated, which they are not. As discussed in Sect. 1, theoretical physical models considered to estimate all nuclear inputs of relevance for the r-process calculations are responsible for the nuclear correlations between the various nuclei involved as well as the between the various properties of interest. For the neutron-rich nuclei relevant to the r-process, for which no experimental information is available, the statistical errors due to variations of model parameters have been shown to be much smaller than the systematic (or model) uncertainties.

5 Similar trends can also be seen in Figs. 2a and b in Zhu et al. (2021).
Figure 21. (Color online) Time evolution of the effective heating rate $Q_{\text{heat}}$ (left column) and the total thermalization efficiency (right column) as defined in eq. 5 for the combined dynamical and secular ejecta for model sfho-135-135 plus M3A8m1a5 (top), sfho-125-145 plus M3A8m3a5-v2 (middle) and sfho-11-23 plus M3A8m3a5-v2 (bottom) when varying the nuclear input between all models listed in Table 2. The gray dashed line in the left panels corresponds to the approximation $Q_0 = 10^{10} \left[ t/1 \text{ day} \right]^{-1.3} \text{ erg/g/s}$. The ratio $Q_{\text{heat}}/Q_0$ is also shown as an insert for $t > 0.1 \text{ d}$ in the left panels, where the line $y = 1$ is indicated by the gray dashed line. See for example Figs. 13, 14, 15 and 16 for the color labels for each nuclear input combination.

(e.g., see Goriely & Capote 2014, who discuss the extrapolation uncertainties of mass models). Therefore, the magnitude of the statistical errors, i.e. the width of the uncertainty distributions often assumed in MC studies, may be significantly overestimated, leading to uncertainty bands spanning several orders of magnitude, as for instance, shown in Figs. 10 and 11 of Mumpower et al. (2016) or Fig. 13 of Nikas et al. (2020). With such large uncertainty bands, it is difficult to obtain detailed information about the overall r-process distribution (i.e. the shape of the r-process peaks and the ratio between them are hidden within the bands). This is not the case when systematically and coherently propagating nuclear uncertainties on the basis of global nuclear models (e.g. see Fig. 18).

As discussed in Sect. 3, not all available global nuclear models are suitable for astrophysical applications. For example, mass models that perform poorly in terms of the rms value with respect to available experimental data should not be included when probing the nuclear uncertainties of the r-process. Works that use what we subjectively deem as “not advisable” models (see also Sect. 4) are indicated in Table 5 to caution the reader that these works might achieve excessively large uncertainty bands in their r-process sensitivity studies. For each study, Table 5 lists the type of ejecta conditions adopted, the number of and origin of the trajectories used, as well as the method applied to vary the nuclear physics input. In particular, the works of Barnes et al. (2021) and Zhu et al. (2021) used single parametrized trajectories for a given $Y_e$ value, fixed expansion time scale and fixed entropy to mimic disk wind conditions. They applied an extensive set of the existing mass models in their input variations, which led to a large uncertainty band spanning up to a factor of 100, in particular for the low-$Y_e$ case shown in Fig. 2 in Zhu et al. (2021). However, if we exclude the nuclear mass models (such as the so-called DZ, UNEDF1, SLy4, TF and ETFSI models), which we judge to inadvisable, their results get closer to ours in terms of the magnitude of the uncertainty stemming from the nuclear mass models. Similarly, for the heating rate shown in Fig. 3 of Zhu et al. (2021), the factor between the maximum and minimum values can be as large as 1000 for the low-$Y_e$ case if all their applied mass models are included, but less than a factor of 100 if only the WS3, HFB-22, HFB-27 and FRDM12 mass models are considered. Similar results are found in Fig. 1 of Barnes et al. (2021) for the nuclear uncer-
tainties on the r-process abundance distribution and heating rates.

Considering now studies using a larger set of trajectories, Eichler et al. (2015) considered 30 trajectories based on a Newtonian hydrodynamical simulation of the low-Y_e dynamical ejecta for their r-process calculations, while Mendoza-Temis et al. (2015) considered 528 low-Y_e relativistic SPH trajectories. Both studied the impact of varying between a few mass models rather similar to those considered here. Their results shown in Figs. 5 and 6 in Eichler et al. (2015) and Mendoza-Temis et al. (2015), respectively, are similar to ours (see in particular Fig. 2e corresponding to the rather similar low-Y_e conditions) in that they predict rather small abundance variations. This is related to the similar nuclear physics input adopted, but also to the fact that they used an ensemble of trajectories instead of single trajectories.

Eichler et al. (2015) also investigated the impact of four fission fragment distribution models on the final r-process abundance distribution. However, they did not implement the SPY or GEF distributions, as we do, but the empirical models of Kodama & Takahashi (1975) and Panov et al. (2001, 2008) and the statistical approach by the ABLA07 code (Kelic et al. 2008; Kelic et al. 2009). Fig. 4b of Eichler et al. (2015) shows an impact in the A ∼ 140 – 150 region comparable to the one observed in our Fig. 12 between the GEF and SPY models. Similarly, Fig. 8 in Vassh et al. (2019) based on a single Y_e < 0.02 dynamical ejecta trajectory, as well as the upper and middle panels of Fig. 3 in Giuliani et al. (2020) based on a similar low-Y_e single trajectory show a significant impact around A ∼ 150 when varying between different models for the fission fragment distributions. The largest divergence can be found between a oversimplified symmetric (Α_{fiss} ≈ \frac{1}{2} Α_{fusion}) relation for the fragments and the GEF fission fragment distributions in Vassh et al. (2019), or the HFB-14 and FRDM+TF fission barriers in Giuliani et al. (2020), both of which are on the same order of magnitude as the deviations we observe between SPY and GEF. Figs. 8 and 9 of Zhu et al. (2021) show the impact of assuming symmetric fragments versus a double peaked Gaussian fission fragment distribution on the heating rates. In order to compare trajectories with the same Y_e and the same nuclear mass model, cases 3 and 4 (blue lines) should be compared, where the relative contribution to the heating rate from α-decays and fission changes between the cases, leading to a discrepancy of a factor of 2, which also impacts the final kilonova light curve shown in their Fig. 11. Similarly, in Figs 11 and 17 of Vassh et al. (2019) a three order of magnitude discrepancy in the heating generated by neutron induced fission is found when varying between symmetric distributions and the GEF fission fragment distributions. In summary, the r-process studies which varied the fission properties in their nuclear physics input showed a significant impact on the shape of the r-process abundance distribution. In particular large deviations were found when the simplistic symmetric fission fragment distributions were applied, and consequently such approximations should be avoided in astrophysical applications. For the works mentioned here, the magnitude and shape of the r-process abundance distribution is generally found to be more robust with respect to changes in the nuclear physics input when a larger set of trajectories are considered and the input is limited to “advisable” models.

Most r-process sensitivity studies have focused on the variation of mass models and neutron capture rates, however, a few have also estimated the impact of varying the theoretical β-decay rates. In particular, Eichler et al. (2015) implemented the RHb+QRPA and FRDM+QRPA rates also applied in our work. Their Figs. 14a and b show that the β-decay rates can impact the shape of the third r-process peak in a way comparable to what we find in our NS-BH scenario (in Figs. 9 and 8). The RHb+QRPA rates reproduce the solar distribution for the low-A end of the peak, while the FRDM+QRPA rates cause deviations from the solar distribution and give rise to a narrower peak. The same trends can also be observed in the lower panel of Fig. 14 in Markiet et al. (2016), Fig. 2 of Caballero et al. (2014) and Fig. 16 of Vassh et al. (2019).

While our approach to estimate the nuclear uncertainties on the r-process yields is only based on theoretical models that have good accuracy and extrapolation reliability (see Sect. 4 for more details), some limitations are present. First of all, due to the limited number of available global nuclear physics models, most of the input sets applied in our r-process calculations are not consistent in terms of, for example, the nuclear mass model and the masses used to calculate the Qβ-values in the β-decay models, or the masses used to calculate the fission properties. These inconsistencies need to be further improved in future nuclear modelling.

5 SUMMARY AND CONCLUSIONS

In this paper, we report an extensive study of the uncertainties related to the theoretical nuclear models which are used as input to r-process nuclear network calculations, and propagate them consistently to the r-process nucleosynthesis to estimate their impact on the abundance distribution and the subsequent radioactive heating rate. Our r-process calculations are based on detailed hydrodynamical models which describe the time evolution of the dynamical and post-merger ejecta including neutrino interactions and viscosity. Our hydrodynamical models do not cover all possible evolutionary paths but include three representative cases of the NS-NS or NS-BH systems, and two subsequent models for the BH-torus system which is expected to form after the merger. These two ejecta components are then combined into the total ejecta. For the NS-NS merger system we use one system with equal-mass NSs, s#o-135-135, and one asymmetrical model, s#o-125-145, which are combined with BH-torus models M3A8m1a5 and M3A8m3a5-v2, respectively. Additionally, we employ one model to describe the dynamical ejecta of a NS-BH merger, model s#o-11-23, which we combine with model M3A8m3a5-v2 (see Table 1). With this setup we study the impact of varying the nuclear physics input on the r-process nucleosynthesis, the heating rate and thermalization efficiency, as well as the predicted age of six metal-poor stars by Th/U cosmochronometry. We vary six nuclear mass models, two frameworks for calculating the radiative neutron capture rates, four β-decay models and two sets of fission barriers and fragment distributions, as detailed in Table 2. Only global mass models that have a rms value smaller than 0.8 MeV are included in this work.

For each nuclear input set, ∼ 200-300 representative trajectories of the full set of ∼ 1000 – 13000 trajectories (depending on the hydrodynamical model applied) are used to...
Table 5. Comparison with previous works: summary of the adopted ejecta conditions, number of trajectories used ($N_{\text{traj}}$), origin of the trajectories (either hydrodynamical simulations or parametrized trajectories), the method used to vary the nuclear physics input and an indication of whether the study includes what we refer to as “advisable” models, see Sect. 3 or 4.5 for details. The ejecta components refer to either the dynamical ejecta of NS-NS or NS-BH mergers (dyn.) or secular wind ejecta in BH-torus remnant systems (wind). Note that the work of Mumpower et al. (2016) summarizes the works of several MC studies.

| Ref.                        | Ejecta comp. | $N_{\text{traj}}$ | Traj. origin | Variation method | “advisable” models |
|-----------------------------|-------------|-----------------|--------------|-----------------|-------------------|
| Barnes et al. (2021); Zhu et al. (2021) | wind, dyn.  | 150-296         | hydro        | systematic      | yes               |
| Mendoza-Temis et al. (2015) | dyn.         | 528             | hydro        | systematic      | yes               |
| Eichler et al. (2015)       | dyn.         | 30              | hydro        | systematic      | only some         |
| Vassh et al. (2019)         | dyn. 1 (k 30)| hydro           | systematic   | only some       |                   |
| Giuliani et al. (2020)      | wind, dyn. 1| hydro & param.  | systematic   | yes             |                   |
| Caballero et al. (2014)     | dyn.         | 1               | hydro        | systematic      | yes               |
| Marketin et al. (2016)      | dyn.         | 1               | hydro        | systematic      | yes               |
| Nikas et al. (2020)         | wind, dyn. 1| hydro           | MC           | only some       |                   |
| Mumpower et al. (2016)      | wind, dyn. 1| hydro & param.  | MC           | yes             |                   |

Figure 22. (Color online) Abundance distributions obtained in eight individual trajectories with different initial neutron fractions (or initial $Y_e$) from model sfho-135-135 (left column) and M3A8m1a5 (right column) using all of the nuclear input sets listed in Table 2. See for example Figs. 13, 14, 15 and 16 for the color labels for each nuclear input combination.

run the r-process nuclear network calculations (see Sect. 3 for more details). In this way, our nucleosynthesis trajectories consistently sample the wide range of thermodynamical conditions encountered at different ejection angles and merger phases. This is in contrast to other sensitivity studies which often only used one single trajectory, or very few trajectories, to represent entire ejecta components (see Sect. 4.5 and Table 5).

The main conclusions from our study can be summarised as follows:

- The uncertainties connected to the nuclear physics input have a minor impact on the global shape of the r-process abundance distribution for the astrophysical scenarios studied here. Our combined ejecta models (consisting of the dynamical NS-NS or NS-BH merger plus the secular BH-torus ejecta) reproduce the solar system distribution well for $A > 90$ and yield a significant amount of Th and U, irrespective of the adopted nuclear physics model. In addition, only small changes of the amount of heavy r-process elements ($X_{A>69}$) and lanthanides plus actinides ($X_{LA}$) are found (see
Table 3) for all model variations. However, when studying the detailed shape of the distribution, a variation between different nuclear physics models can give a significant (local) impact (see Fig. 19). When fission plays an important role (i.e. for the NS-BH case), the largest impact on the abundance distribution and the heating rate is found in connection with the fission barrier height and fragment distribution.

- The position, shape and width of the r-process peaks vary with the nuclear physics input used, but also with the ejecta model. In particular, when mass model HFB-31 is applied, an additional structure at $A \sim 130 - 140$ appears, and for BH-torus model M3A8m3a5-v2 a very narrow peak around $A \sim 132$ is formed, which is not observed for the other BH-torus or dynamical models. For the high-$X_n$ (e.g., low-$Y_e$) conditions in the NS-BH merger, the width of the third r-process peak is very sensitive to the adopted $\beta$-decay rates, where the RHB+RQRPA rates of Marketin et al. (2016) leads to better agreement with the solar r-process distribution, as also found in in other studies, see Sect. 4.5.

- While globally all nuclear models give rise to a rather similar ejecta composition, deviations up to a factor $\sim 20$ can be found for some specific individual abundances of elements with $A > 90$, in particular around the second and third r-process peaks (the latter being most prominent for the NS-BH merger scenario). The factor between the largest and smallest yields of actinides ranges between 5 and 7.

- The radioactive heating rate before thermalization is found to be relatively insensitive (within a factor of $\lesssim 2$) to variations of the nuclear physics input at early times ($t \lesssim 10$ d). However, larger deviations are found in particular related to the contribution from fission in cases where heaviest elements are produced (i.e. for the NS-BH case at $t \gtrsim 5$ d). The thermalization efficiency introduces an additional spread between different nuclear physics models, particularly at late times when alpha-decay and spontaneous fission become important.

- We find a similar order of magnitude for the uncertainties due to the nuclear physics input when we compare our results to the works of others which also systematically varied the nuclear input between global models similar to the ones applied here. A larger impact, up to a factor of 100 on individual $A > 90$ r-process nuclei, and 1000 on the heating rates can be found when applying global models which we do not recommend for astrophysical applications due to their poor performance in accurately reproducing measured data (Barnes et al. 2021; Zhu et al. 2021), or when considering MC-type methods (e.g., Mumpower et al. 2016, and references therein).

- For the astrophysical scenarios studied here, the nuclear physics uncertainties are typically small compared to variations related to the different ejecta components. Moreover, they are also small (or at most similar) compared to the variations encountered when using different disk masses BH masses, and BH spins in BH-torus simulations (e.g., Wu et al. 2016; Just et al. 2021b) or different EoSs in NS-NS merger simulations (Kullmann et al. 2021; Sekiguchi et al. 2015; Radice et al. 2016). This circumstance strengthens the credibility of nucleosynthesis analyses based on hydrodynamical models of these systems, and it lends further support to the notion that NS mergers can be significant sources to r-process elements in the Universe.

- For the stellar U/Th cosmochronometry age estimates, the uncertainties connected to the nuclear physics input are still larger than the variations associated with changing the hydrodynamical model (for the cases studied here). The mean age inferred by our method for the six metal poor stars varies between $11 \pm 2$ and $19 \pm 2$ Gyr for stars CS22892-052 and CS29497-004, respectively. So far, the observational uncertainties (on the order of $\sim 3-7$ Gyr) remain significantly larger than the nuclear physics ones.

It is difficult to pin down a single nucleus (or a few nuclei) having a dominant impact on the nuclear r-process uncertainties. First, because when changing the nuclear input from one model to another, many nuclei are affected in a systematic way (in contrast to other types of sensitivity studies which neglect systematic correlations and change, for example, the neutron capture rate of individual reactions randomly within a given range). Second, because the r-process conditions can vary between the astrophysical scenarios, the significance of a nuclear process can also vary, which would change the sensitivity resulting from a specific nuclear mass region.

Therefore, efforts on the experimental as well as theoretical side will have to continue to systematically improve the amount of data available and the description of nuclear structure, reactions and radioactive decay of neutron-rich nuclei in the foreseeable future. In particular, a future aim should be to develop fully consistent models for all nuclear physics properties (e.g., masses, $\beta$-decay; fission...) required as input for r-process calculations. Similarly, the push towards improving hydrodynamical simulations of the NS-NS or NS-BH merging systems covering the dynamical as well as post-merging phases will greatly improve our understanding of the conditions for the r-process. In particular, questions regarding the mass, velocity, entropy, and neutron-richness of the various ejecta components need to be further resolved. With continuous advancements on the nuclear and astrophysical side, systematic studies of the nuclear physics impact will continue to be important in order to quantify the uncertainties of r-process yields and their corresponding production of decay heat.

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DATA AVAILABILITY
The data underlying this article will be shared on reasonable request to the corresponding author.

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