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MESA and NuGrid Simulations of Classical Nova Outbursts and Nucleosynthesis

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Abstract. Classical novae are the results of surface thermonuclear explosions of hydrogen accreted by white dwarfs (WDs) from their low-mass main-sequence or red-giant binary companions. Chemical composition analysis of their ejecta shows that nova outbursts occur on both carbon-oxygen (CO) and more massive oxygen-neon (ONe) WDs, and that there is cross-boundary mixing between the accreted envelope and underlying WD. We demonstrate that the state-of-the-art stellar evolution code MESA and post-processing nucleosynthesis tools of NuGrid can successfully be used for modeling of CO and ONe nova outbursts and nucleosynthesis. The convective boundary mixing (CBM) in our 1D numerical simulations is implemented using a diffusion coefficient that is exponentially decreasing with a distance below the bottom of the convective envelope. We show that this prescription produces maximum temperature evolution profiles and nucleosynthesis yields in good agreement with those obtained using the commonly adopted 1D nova model in which the CBM is mimicked by assuming that the accreted envelope has been pre-mixed with WD's material. In a previous paper, we have found that ^{3}He can be produced *in situ* in solar-composition envelopes accreted with slow rates ($\dot{M} < 10^{-10}\,M_\odot$/yr) by cold ($T_{\rm WD} < 10^7$ K) CO WDs, and that convection is triggered by ^{3}He burning before the nova outburst in this case. Here, we confirm this result for ONe novae. Additionally, we find that the interplay between the ^{3}He production and destruction in the solar-composition envelope accreted with an intermediate rate, e.g. $\dot{M} = 10^{-10}\,M_\odot$/yr, by the $1.15\,M_\odot$ ONe WD with a relatively high initial central temperature, e.g. $T_{\rm WD} = 15\times10^6$ K, leads to the formation of a thick radiative buffer zone that separates the bottom of the convective envelope from the WD surface.

1. Introduction

MESA is a collection of Fortran-95 **M**odules for **E**xperiments in **S**tellar **A**strophysics. Its main module `star` can be used for 1D stellar evolution simulations of almost any kind (numerous examples are provided by Paxton et al. (2011, 2013) and on the MESA website `http://mesa.sourceforge.net`). For instance, `star` can compute without any interruption the evolution of a solar-type star from the pre-MS phase through

the He-core flash and thermal pulses on the asymptotic giant branch towards the WD cooling. Only a few codes can do such computations. Other MESA modules provide `star` with state-of-the-art numerical algorithms, e.g. for adaptive mesh refinement and timestep control, atmospheric boundary conditions, and modern input physics (opacities, equation of state, nuclear reaction rates, etc.)

The nucleosynthesis calculations presented in this work are made by the post-processing code PPN (developed inside the NuGrid research framework, Herwig et al. 2008), where the input data of stellar structure (e.g., from MESA models) are processed using a comprehensive list of nuclear species and reaction rates. The network can include more than 5000 species, between H and Bi, and more than 50000 nuclear reactions. A self-controlled dynamical network defines the actual numbers of species and reactions considered in calculations, based on the strength of nucleosynthesis fluxes. For the complete post-processing of the full MESA nova models, we use the multi-zone parallel frame of PPN (MPPNP), whereas for the simulations based on a single-zone trajectory we use the serial frame (SPPN). The two frames use the same nuclear physics library and the same package to solve the nucleosynthesis equations (for details, go to `http://www.nugridstars.org`).

We have prepared shell scripts, template MESA inlist files, and a large number of initial WD models aiming to combine MESA and NuGrid into an easy-to-use Nova Framework. This new research tool can model nova outbursts and nucleosynthesis occurring on CO and ONe WDs using up-to-date input physics and a specified nuclear network for a relatively large number (up to a few thousands) of mass zones covering both the WD and its accreted envelope. Nova simulation results can be analyzed using animations and a variety of plots produced with NuGrid's Python visualization scripts. This article reports the new results obtained with the Nova Framework and demonstrates some of its capabilities.

2. One-Dimensional Nova Models With Convective Boundary Mixing (CBM)

To be consistent with observations, a realistic nova model should assume that the accreted material has solar composition (for the solar metallicity) and that it is mixed with WD's material before or during its thermonuclear runaway. Recent two- and three-dimensional nuclear-hydrodynamic simulations of a nova outburst have shown that a possible mechanism of this mixing are the hydrodynamic instabilities and shear-flow turbulence induced by steep horizontal velocity gradients at the bottom of the convection zone triggered by the runaway (Casanova et al. 2010, 2011a,b). These hydrodynamic processes associated with the convective boundary lead to convective boundary mixing (CBM) at the base of the accreted envelope into the outer layers of the WD. As a result, CO-rich (or ONe-rich) material is dredged-up during the runaway. In our 1D MESA simulations of nova outbursts, we use a simple CBM model that treats the time-dependent mixing as a diffusion process. The model approximates the rate of mixing by an exponentially decreasing function of a distance from the formal convective boundary,

$$D_{\rm CBM} = D_0 \exp\left(-\frac{2|r - r_0|}{f H_P}\right), \tag{1}$$

where H_P is the pressure scale height, and D_0 is a diffusion coefficient, calculated using a mixing-length theory, that describes convective mixing at the radius r_0 close to the

boundary. In this model f is a free parameter, for which we use the same value $f = f_{\rm nova} = 0.004$ that we used in our CO nova simulations in Paper I (Denissenkov et al. 2013). For a physical motivation to model the CBM with the prescription (1), see Paper I. Our MESA nova models with the CBM have been post-processed with the MPPNP code, and the resulting final abundances have been compared with those obtained for the corresponding nova models without CBM but with the 50% pre-mixed accreted envelopes. The comparison between the final abundances shows a very good agreement for both the CO and ONe nova models (the left panel of Fig. 1 and Fig. 1 in Denissenkov et al. 2012; we disavow our conclusion made in that paper that it was not true for CO novae). This gives a support to the widely-adopted 1D nova model in which the CBM is mimicked by assuming that the accreted envelope has been pre-mixed with WD's material.

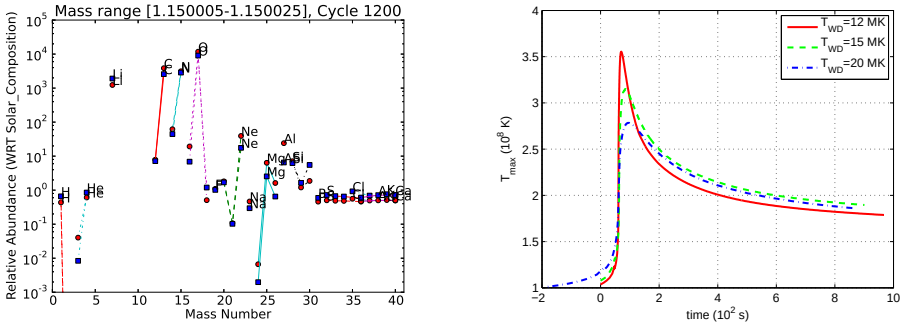

Figure 1. Left panel: A comparison of final solar-scaled abundances of stable isotopes from two of our 1.15 $M_\odot$ CO nova simulations with $T_{\rm WD} = 12$ MK and $\dot{M} = 2 \times 10^{-10}\ M_\odot$/yr. The red circles are the results obtained with the 50% pre-mixed initial abundances in the accreted envelope, while the blue squares represent the case with the solar-composition accreted material and convective boundary mixing (CBM) modeled using the same method and CBM parameter $f_{\rm nova} = 0.004$ that we used in the 1.2 $M_\odot$ CO nova model in Paper I. Right panel: $T_{\rm max}$-trajectories from three of our 1.3 $M_\odot$ 50% pre-mixed ONe nova models computed for the same accretion rate, $\dot{M} = 2 \times 10^{-10}\ M_\odot$/yr, but different WD's initial central temperatures. The initial isotope abundances are those of the Barcelona group (José et al. 1999, 2001).

3. Comparison of the Results of SPPN and MPPNP Simulations

Single-zone post-processing calculations of nova nucleosynthesis with the NuGrid code SPPN are done for a mass zone in a nova envelope where the temperature profile has its maximum, $T = T_{\rm max}$ (usually, near the core-envelope interface). For this, the temporal variations of $T_{\rm max}$ and its corresponding density, called "trajectories", are extracted from MESA models (e.g., the right panel of Fig. 1). The SPPN code runs much faster than MPPNP, therefore it can be used for a comprehensive numerical analysis of parameter space, when the relevant isotope abundances and reaction rates are varied within their observationally and experimentally constrained limits. A comparison between the final abundance distributions in Fig. 2 shows a qualitative agreement between the results from the single-zone $T_{\rm max}$-trajectories (the left panel) and from their correspond-

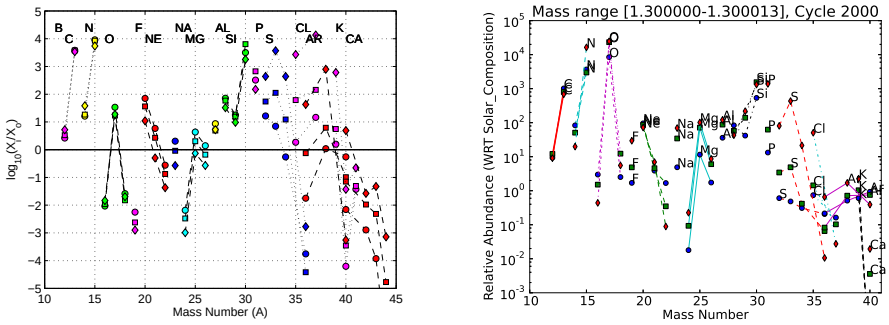

Figure 2. Left panel: the final solar-scaled abundances of stable isotopes calculated with the SPPN code using the trajectories from the right panel of Fig. 1 that correspond to the three different WD's initial central temperatures: $T_{\rm WD}$ = 12 MK (diamonds), 15 MK (squares), and 20 MK (circles). Right panel: the same final abundances, but calculated with the MPPNP code using the corresponding full MESA models and averaged over the indicated mass range in the expanding nova envelope.

ing multi-zone complete models (the right panel). Indeed, the abundance patterns for different groups of isotopes look similar. The main quantitative difference is the more efficient production toward heavier species in the first case, where O is more depleted, while Ar and K isotopes[1] are more efficiently made. This difference is caused by the fact that in the multi-zone post-processing simulations convective mixing reduces an "average temperature" at which the nucleosynthesis occurs and it also constantly replenishes the hydrogen fuel burnt at the base of the envelope by bringing it from its outer parts, where $T \ll T_{\rm max}$. In general, the results in Fig. 2 show how the increase of the $T_{\rm max}$ peak value (the right panel of Fig. 1) changes the relative abundance distribution. We conclude that SPPN nucleosynthesis simulations with nova $T_{\rm max}$-trajectories provide a proper qualitative indication of the behavior of their corresponding complete MPPNP simulations. However, they can be used only as a diagnostic for nova nucleosynthesis, e.g. in reaction rate sensitivity studies.

4. Effects Caused by ^{3}He Burning

In Paper I, we have found, for the first time, that in the extreme case of a very cold CO WD, e.g. with $T_{\rm WD}$ = 7 MK, accreting solar-composition material with a very low rate, say $\dot{M} = 10^{-11}\,M_\odot$/yr, the incomplete pp I chain reactions lead to the *in situ* synthesis of ^{3}He in a slope adjacent to the base of the accreted envelope and that the ignition of this ^{3}He triggers convection before the major nova outburst. The ^{3}He burning continues at a relatively low temperature, $T \approx 30$ MK, approximately until its abundance is reduced below the solar value, only after that the major nova outburst ensues triggered by the reaction ^{12}C(p,γ)^{13}N. Although this is an interesting variation of the nova scenario,[2] because the CO enrichment of the accreted envelope is produced by the ^{3}He-driven

[1]The Barcelona composition specifies the initial abundances only for isotopes lighter than Ca.

[2]Initially, ^{3}He was considered as the most likely isotope to trigger a nova outburst by Schatzman (1951).

CBM in this case, its observational frequency is expected to be very low (Paper I). Later, we have confirmed this result for ONe novae (Fig. 2 in Denissenkov et al. 2012). Furthermore, we have found that in the 1.15 $M_\odot$ ONe WD with a relatively high initial central temperature, $T_{\rm WD} = 15$ MK, accreting the solar-composition material with the intermediate rate, $\dot{M} = 10^{-10}\,M_\odot$/yr, the interplay between the ^{3}He production and destruction in the vicinity of the base of the accreted envelope first leads to a shift of $T_{\rm max}$ away from the core-envelope interface followed by the formation of a thick radiative buffer zone that separates the bottom of the convective envelope from the WD surface (Fig. 3 in Denissenkov et al. 2012). This result is obtained only for the case when an ONe WD accretes solar-composition material and it almost disappears in the models with the pre-mixed accreted envelopes. Given that the formation of the radiative buffer zone is revealed in the computations with the more realistic nova model parameters, such cases can probably be observed. We defer a more detailed study of this peculiar case and its possible consequences to a future work. In particular, it would be interesting to see if the CBM can cross the buffer zone and reach the WD.

5. Conclusion

We have created the Nova Framework that allows to simulate the accretion of H-rich material onto a white dwarf (WD) leading, for a suitable set of initial parameters, to a nova outburst, and to post-process its accompanying nucleosynthesis. The Nova Framework combines the state-of-the-art stellar evolution code MESA and post-processing nucleosynthesis tools of NuGrid. It includes a number of CO and ONe WD models with different masses and central temperatures (luminosities) that can be used in simulations of nova outbursts. The use of the Nova Framework is facilitated by a number of shell scripts that do the routine job necessary to coordinate the operation of the MESA and NuGrid codes.

Within the Nova Framework project, we have provided a large set of nucleosynthesis calculations for nearly 50 CO and ONe nova models at the solar metallicity ($Z = 0.02$) so far. To verify our calculations, we have compared their results with those published in the literature for similar nova models. The comparison shows a very good qualitative agreement.

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