

Nucleosynthesis simulations for a wide range of nuclear production sites from NuGrid

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Simulations of nucleosynthesis in astrophysical environments are at the intersection of nuclear physics reaction rate research and astrophysical applications, for example in the area of galactic chemical evolution or near-field cosmology. Unfortunately, at present the available yields for such applications are based on heterogeneous assumptions between the various contributing nuclear production sites, both in terms of modeling the thermodynamic environment itself as well as the choice of specific nuclear reaction rates and compilations. On the other side, new nuclear reaction rate determinations are often taking a long time to be included in astrophysical applications. The NuGrid project addresses these issues by providing a set of codes and a framework in which these codes interact. In this contribution we describe the motivation, goals and first results of the NuGrid project. At the core is a new and evolving post-processing nucleosynthesis code (PPN) that can follow quiescent and explosive nucleosynthesis following multi-zone 1D-stellar evolution as well as multi-zone hydrodynamic input, including explosions. First results are available in the areas of AGB and massive stars.

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1. Introduction

Nuclear astrophysics combines nuclear physics of astrophysical relevance with the simulation of nuclear production sites in stellar evolution and explosions, and ultimately with abundance observations in stars and galaxies and measurements in pre-solar grains. Numerous compilations of yield data, for applications such as chemical evolution of galaxies, have been presented, based on different modeling assumptions. For example, in the area of massive stars the compilation of Woosley & Weaver (1995) provides yields which is based on solving a nuclear network together and in lock-step with the stellar evolution code. A similar approach is applied for AGB star yields [8, 10], although yields based on synthetic models are also still in use [11]. The latter was justified by the significant labour involved in full stellar evolution tracks of the advanced phases of stellar evolution, where most of the interesting nucleosynthesis takes place. It is largely for this reason that we still don't have yield tables that cover low-mass *and* massive stars (including explosive yields) for a meaningful range of metallicities and both light *and* heavy elements with internally consistent physics assumptions, including the nuclear physics data. However, such comprehensive yield data is required, for example in near-field cosmology applications [16, 6].

In addition, new results, for example on the hydrodynamic nature of convective boundary mixing (Woodward et al., this vol. and [12]), need to be included in new yield calculations as quickly as possible to make them available for comparison with observations. Finally, the nuclear physics community needs to prioritize their efforts through the ability to run numerical nucleosynthesis experiments in realistic stellar production environments.

In order to address these issues we have pooled capabilities and expertise in the nucleosynthesis grid (NuGrid) collaboration to create a new simulation library and nucleosynthesis code capability. In this paper we describe our approach and report first results, for example from AGB s process and massive star nucleosynthesis. Other results relating to the NuGrid project have been presented at this conference by Hirschi et al., Pignatari et al., Fryer et al., Diehl et al., Hungerford et al. and Rockefeller et al. .

2. NuGrid nucleosynthesis post-processing

We have developed a new post-processing nucleosynthesis (PPN) code, and we are developing a stellar evolution and explosion (SEE) database, including an interface that allows these two components to communicate efficiently. The ultimate goal is to combine these two tools to create the needed comprehensive and internally consistent yields tables. The design goals of the PPN codes are (1) a capability of post-processing a wide range of thermodynamic environments from both 1D stellar evolution codes and trajectories from hydro-simulations (explosions and stellar hydro, both grid and particle), (2) comprehensive yet flexible nuclear physics input, and (3) to match resolution, detail, accuracy and precision of third dredge-up simulations, observations and nuclear physics.

The core unit of the PPN code implementation is a nuclear network kernel that consists of a physics package and a solver package. The nuclear network kernel evolves one nuclear network cell over one time step. There are three drivers that use the same network kernel. The single-zone driver (SPPN) is used for simple one-zone network experiments with either analytic, algorithmic or tabulated thermodynamic input. The multi-zone driver (MPPN) post-processes the output of

one-dimensional spherically symmetric stellar evolution codes, while the trajectory driver (TPPN) deals with trace particle data from hydrodynamic simulations.

The nuclear physics package includes most major nuclear data compilations, i.e. Basel reaclib [14], Kadonis [5], NACRE [2], Illiadis et al. (2001, [9]), Cauhglan & Fowler (1988, [4]), the nuclear data online interface Bruslib [1], Oda et al. (1994, [13]) and Fuller et al. (1985, [7]). The network includes NSE with T-dependent partition functions and mass excesses from reaclib and Coulomb screening from Calder et al. (2007, [3]). The network is dynamically built in two steps. In a first configuration step the master set of isotopes out of a maximum of 5180 is selected using simple configuration instructions. Based on this master set the actual network is adjusted dynamically in size for each network kernel calculation, so that the solution in every network cell is performed for the optimal selection of isotopes. The solver package relies at this time on a Newton-Raphson, fully implicit implementation with full precision control and adaptive sub-time stepping. We are also implementing a variable order method for improved accuracy [15]. The multi-zone and trajectory drivers are parallelized through a simple master-slave strategy, implemented in the distributed memory paradigm. The parallel MPPNP driver has been run on up to 150 cores, although in most practical applications we are running post-processing grids of ~ 250 shells on 60-80 cores. The MPPNP drivers provides three grid options: static, input grid or adaptive grid.

The interface to the stellar evolution and explosion data is defined through the custom library USEEPP¹ built on top of the platform independent hdf5² standard. The SEE database is populated with low-mass tracks with the EVOL code (Pignatari et al., this vol.) and with tracks from the Geneva code (Hirschi et al., this vol.) and the Tycho code [18] for massive stars. Within the physics options implemented in these codes we are calibrating the free parameters to obtain the largest possible internal consistency (Fig. 1). Explosion simulations in the SEE database are provided as described in Fryer et al. (this vol.).

One potential problem with the post-processing approach is the need to exactly match nuclear reactions that produce the majority of the nuclear energy in the stellar evolution and post-processing code. We have a special interface in the physics package to either reproduce exactly the same reaction rate source as used in the stellar evolution code, or to introduce the same subroutine with the same interpolation or fit formula evaluation algorithm as used in the stellar evolution calculation. In addition, we save up to ten control abundances that are primarily linked to the energy produc-

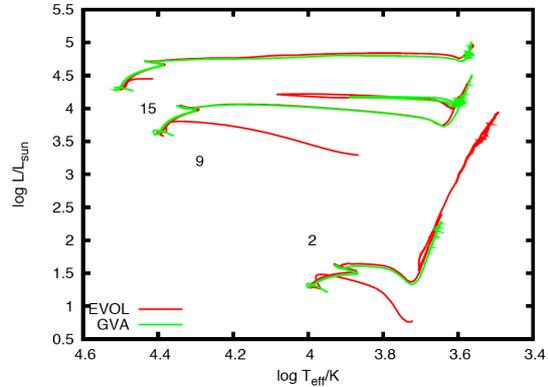


Figure 1: Stellar evolution tracks from EVOL and GVA (Geneva code) for different masses as indicated, without rotation, identical initial composition and an overshoot parameter ($f_{ov} = 0.014$ for EVOL and $\alpha_{ov} = 0.2$ for GVA) that has been chosen so that the width and duration of the main-sequence match.

¹USEEPP = Unified Stellar Evolution and Explosion Post-Processing

²<http://www.hdfgroup.org/HDF5>

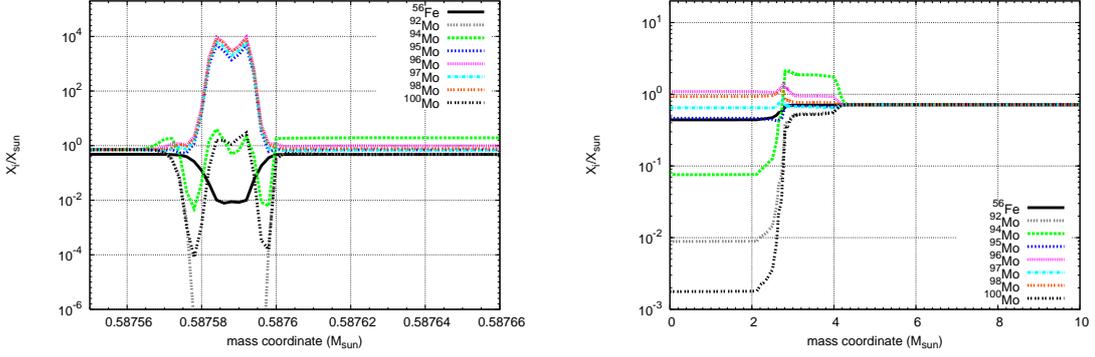


Figure 2: Post-processing results for the Mo isotopes and the s-process seed ^{56}Fe at the end of the interpulse ^{13}C -pocket nucleosynthesis (left) as in Pignatari et al. (this vol.) and in He-core burning in a $15M_{\odot}$ model (right) as described in more detail in Hirschi et al. (this vol.)

tion in the USEEPP format, and monitor any differences that may develop between the original and post-processing nucleosynthesis. Another problem may be to correctly map the original stellar evolution or explosion calculation into the post-processing code. Through our USEEPP IO library all thermodynamic and mixing data in all mass zones and all time steps of all tracks are saved, which takes on average 5GB per full stellar evolution track. We are then able to either post-process on the original stellar evolution grid, or accomodate special grid requirements of the nucleosynthesis. Thus, our post-processing approach is accurate with the added benefit of additional grid options, updated nuclear physics and optionally higher-order solvers. The results are as reliable as yields calculated with an extra nucleosynthesis step inlined into the stellar evolution simulations, with a larger network than used for the energy generation feeding into the stellar structure solver [17, 10]. Contrary to the latter approach we can rerun our post-processing with any nuclear physics input at minimal human labour cost. This method is affordable, with a full post-process run of one stellar evolution track sequence (10^5 time steps, ~ 300 pp grid zones) taking 2 days on $\sim 60 \dots 80$ cores.

We have so far populated the SEE database with both low-mass and massive star tracks (Fig. 1). A major advantage of our approach is the ability to calculate the nucleosynthesis in both regimes with the same MPPNP code and the same nuclear physics data. At solar-like metal content s-process contributions to Mo come from AGB stars. However, as discussed in this volume by Hirschi et al., models of very low metal content with rotation may produce significant amounts of s-process elements between Sr and Ba, including Mo. Fig. 2 demonstrates by example of Mo nucleosynthesis in an AGB and a massive star environment how we will use our NuGrid to investigate nucleosynthesis in a comprehensive and consistent way.

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