

# Density Conversion between 1D and 3D Stellar Models with <sup>1D</sup>MESA2HYDR

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## Abstract

We present <sup>1D</sup>MESA2HYDRO<sup>3D</sup>, an open-source, Python-based software tool that provides an accessible means of generating physically motivated initial conditions (ICs) for hydrodynamical simulations from 1D stellar structure models. We test <sup>1D</sup>MESA2HYDRO<sup>3D</sup> on five stellar models generated with the MESA stellar evolution code and verify its capacity as an IC generator with the Phantom smoothed particle hydrodynamics code. Consistency between the input density profiles, the <sup>1D</sup>MESA2HYDRO<sup>3D</sup>-rendered particle distributions, and the state of the distributions after evolution over 10 dynamical timescales is found for model stars ranging in structure and density from a radially extended supergiant to a white dwarf.

Unified Astronomy Thesaurus concepts: Astronomy software (1855); Stellar evolutionary models (2046); Stellar structures (1631)

#### 1. Introduction

The objective of stellar modeling is to reproduce the observed characteristics of stars with as much fidelity to physical reality as possible. Given unlimited time and computational resources, we would simulate entire stellar life cycles in rigorous, 3D detail; however, it is not currently computationally feasible to compute the evolution of a star particle by particle in 3D. Because of this practical limitation, 1D stellar structure and evolution codes (SSECs) are used to model the secular evolution of stars over astronomical timescales (e.g., DSEP, Y<sup>2</sup>, BaSTI, MESA, and many others; Demarque et al. 2004; Pietrinferni et al. 2004; VandenBerg et al. 2006; Cordier et al. 2007; Dotter et al. 2008; Paxton et al. 2018). Models of this type are sufficient and highly effective for a wide range of applications, but they are not well suited to some important, intrinsically 3D phenomena. Processes such as dynamical stellar behavior, stellar interactions, mergers, and convection cannot be captured realistically using 1D codes. Rather, astrophysical problems of this nature are best approached using full 3D modeling for isolated scenarios or on shorter physical timescales. The appropriate tool for such problems is a 3D hydrodynamics code (Springel 2005; Mohamed et al. 2012; Price 2012; Hopkins 2015; Booth et al. 2016; Goldbaum 2017; Ramstedt et al. 2017; Price et al. 2018).

With the many SSECs now in use, astronomers can produce models that take into account a wide range of physical processes, including elemental diffusion, gravitational settling, fine-tuning of mixing events, and elaborate meshes for specifying the initial abundances of over 50 elements individually. The highly customizable nature of these codes makes them especially powerful, as the user may designate any number of physical attributes (mass, abundances, equation of state, opacity tables, mixing prescriptions) and recover the surface or structural state of the model star at any point in evolutionary time.

To make them as realistic as possible, SSECs integrate externally generated grid data, including opacities, model atmospheres, and mixing specifications, which are calculated using 3D

simulations or other more sophisticated methods (Iglesias & Rogers 1996; Hauschildt et al. 1999; Ferguson et al. 2005; Trampedach 2007; Arnett et al. 2015; Magic et al. 2015). Fundamentally, however, SSECs are still based on a 1D formalism, and as such are not capable of capturing particledriven processes themselves. Rather, the modeling techniques best suited to these tasks are those that compute the properties of large numbers of fluid elements over short timescales in three dimensions; these include hydrodynamics codes such as GAD-GET-2, AREPO, AstroBEAR, Phantom, and many others (Springel 2005, 2011; Cunningham et al. 2009; Hopkins 2015; Price et al. 2018). Thorough reviews of the hydrodynamical modeling landscape and summaries of the capabilities and mechanics of many such codes are provided in, e.g., Rosswog (2009), Springel (2010), Price (2012), and Goldbaum (2017).

A critical aspect of hydrodynamical modeling is the specification of the initial distributions in mass, energy, and other physical quantities at the onset of the simulation. Often, the initial mass distribution that represents a star or stellar atmosphere is obtained by generating an arbitrary particle distribution that follows a 1/r profile (Price 2012). While sometimes appropriate and sufficient, this choice is often made ad hoc and may not reflect the actual distribution of material in a star very accurately.

The need for and feasibility of other techniques to construct initial conditions (ICs) with more physical fidelity has been recognized, for instance, in the work of Pakmor et al. (2012), who showed that a method for building a 3D configuration using concentric, shellular distributions of particles was effective for modeling white dwarfs. More recently, Ohlmann et al. (2017) demonstrated that a 1D density profile generated directly with MESA (Paxton et al. 2018) could be used to construct ICs for 3D hydrodynamical models of red giants. This technique has inspired the development of our package. <sup>1D</sup>MESA2HYDRO<sup>3D</sup> is an open-source IC generator for

hydrodynamical simulations that use equal-mass particles.

Generalizing and extending the work of Ohlmann et al. (2017), <sup>1D</sup>MESA2HYDRO<sup>3D</sup> constructs a particle distribution based directly on an SSEC-generated radial density profile provided by the user. Because it samples a stellar structure model directly, <sup>1D</sup>MESA2HYDRO<sup>3D</sup> makes it easier to incorporate the customizable physics of 1D SSECs into 3D hydrodynamical simulations.

In this paper, we present the release of <sup>1D</sup>MESA2HYDRO<sup>3D</sup>, describe our methods, and demonstrate consistency between MESA density profiles and the particle distributions <sup>1D</sup>MESA2HYDRO<sup>3D</sup> generates from them. We test our package on five model stars with diverse structures encompassing a density range of 18 dex. We demonstrate that the tool can effectively render density profiles as computationally tractable, physically adherent particle distributions across a broad span of parameter combinations. We directly verify <sup>1D</sup>MESA2HYDRO<sup>3D</sup>'s utility as an IC generator using the Phantom smoothed particle hydrodynamics (SPH) code.

## 2. MESA Models as ICs

The package <sup>1D</sup>MESA2HYDRO<sup>3D</sup> can convert any radial density profile that is smooth, physically reasonable, and formatted compatibly. However, we have focused our efforts toward integration with the MESA code for a few reasons: (1) the MESA community is large, spans a broad range of interests, and adheres to an open-source ethos; (2) the MESA code is under active development, with new releases every few months; and (3) MESA has the highest degree of customizability of any stellar evolution code. The user can control thousands of parameters, many of which impact the structural aspects of the model star. The preservation of such effects is the primary benefit <sup>1D</sup>MESA2HYDRO<sup>3D</sup> provides over less complicated methods for prescribing density profiles in hydrodynamical ICs.

MESA is a suite of open-source, thread-safe libraries developed in Fortran 95. It contains distinct modules for handling the equations of state, opacity, nuclear reaction rates, diffusion data, and atmospheric boundary conditions. Each module is a separate library with its own public interface, supports shared memory parallelism based on the OpenMP application program interface, and employs adaptive mesh refinement and time-step control. Extensive testing of MESA indicates that the code effectively calculates the evolution of stars over a wide range of masses (from sub-neptunes to  $M \sim 1000 M_{\odot}$ ) and over evolutionary phases spanning from the pre-main sequence to the onset of core collapse in high-mass stars or the white dwarf stage in lower-mass stars. Detailed information on the workings of MESA is available in several instrument papers, including Paxton et al. (2011, 2013, 2015, 2018).

The physical attributes of a stellar model are specified in MESA via a central control file called an "inlist." This contains all modeling, physical, and plotting controls used in the evolutionary run. The public release of <sup>1D</sup>MESA2HYDRO<sup>3D</sup> includes copies of the inlists used to generate our test stars, where variable names have the same definitions as in MESA version 10398.

Throughout the course of a run, MESA generates "profile" files, or snapshots of the state of the star from core to surface, as a function of radius (equivalently, mass contained). The user can control the output frequency of these snapshots. Meanwhile, a "history" file tracks the secular evolution of the global state variables—mass, radius, effective temperature, average density, etc., and the quantities derived from these—as a function of time. One can thus recover the structure during any evolutionary phase by specifying stop conditions that correspond to the desired physical criteria. To obtain a structural model of a thermally pulsing asymptotic giant branch (TP-AGB) star, for example, the user can simply specify that MESA should terminate evolution during a thermal pulse (e.g., Molnár et al. 2019).

The input MESA profiles must have a particular data organization to be compatible with <sup>1D</sup>MESA2HYDRO<sup>3D</sup>. For reference, we include the complete glossaries of MESA parameter defaults (as they appeared in MESA version 10398), as well as the particular settings used to generate our test suite for each of the four standard MESA control lists: "controls," "star\_job," "history\_columns," and "profile\_columns." The last of these dictates the data format that should be used when generating profiles intended for use with our package. The user may also provide a stellar structure model generated by another SSEC as long as it is in a format understood by <sup>1D</sup>MESA2HYDRO<sup>3D</sup>. For instance, the data columns in a compatible model must adhere to the MESA naming conventions, using, e.g., "logR" as the column name for  $(\log_{10})$  radius. The <sup>1D</sup>MESA2HYDRO<sup>3D</sup> User's Guide gives an example of a correctly formatted input profile and provides the column header keywords ("logR," "mass," "logRho," etc.) needed to build one's own input model, if desired. The manual also provides more detail on MESA control files. It is freely available by request from the authors prior to public release. The physical quantities required by <sup>1D</sup>MESA2HYDRO<sup>3D</sup>

The physical quantities required by <sup>1D</sup>MESA2HYDRO<sup>3D</sup> are, minimally, mass, density, pressure, and internal energy as a function of radius. The latter two are necessary to ensure piecewise compatibility between the equations of state in the 1D and 3D models and to compute smoothing lengths for the SPH particles.

MESA inlists corresponding to the five stars tested in this paper are included with the package. These serve as a useful starting point, but users should change the parameters to suit their needs. Some knowledge of the appropriate astrophysical choices is required in order to generate reasonable models.

#### 3. Methods

The backbone of the 1D to 3D mapping is the conversion of discrete r,  $\rho(r)$  data to a set of mass and radial coordinates that can be reinterpreted as particle distributions. These are referred to henceforth as N, R coordinates, abbreviated for "number" and "radius."

The radial coordinate *R* represents the value at which a particular shell must be located relative to the stellar core in order to recast the mass contained in the region  $(r_u - r_l)$  equivalently as a distribution of discrete particles covering the surface of a sphere. The *R* coordinates are actually midpoint values  $r_{\text{mid}} = (r_l + r_u)/2$ , where  $r_l$ ,  $r_u$  are the inner and outer bounds, respectively, on the mass region to be mapped. The number *N* corresponds to an integer used by the Hierarchical Equal Area isoLatitude Pixelization (HEALPix) spherical tessellation algorithm to dictate the total number of particles  $n_p$  distributed over a single spherical shell (Górski et al. 2005). This coordinate, in conjunction with the user's choice for particle mass  $m_p$ , controls mass.

For all models in the current test suite, the same value of N is used for every shell; in a sense, this makes the choice of N a global parameter. However, it is prudent to treat N as a local

coordinate because it is set independently per shell and the value of R depends on it. As such, it is possible to create particle distributions with varying N or stitch together coordinate files parameterizing different regions of the same model using distinct N values, though we do not do so here.

The calculation of the *R* coordinates relies on a root-finding procedure that searches the 1D profile data passed initially; as such, <sup>1D</sup>MESA2HYDRO<sup>3D</sup> works best for profiles that are relatively smooth. Though the algorithm can handle density profiles that are nonmonotonic, it is slower in these regions. The number of *N*, *R* coordinates generated for a given density profile corresponds to the number of shells used in the 3D distribution. Shell counts on the order of a few hundred to a few thousand will produce distributions comprising particle numbers that are manageable for most hydrodynamics codes.

For a hydrodynamical simulation to be physically meaningful, it is important that the ICs do not produce preferred directionality or organized motion when the simulation evolves (Mohamed 2009). One method for building stellar particle distributions with the appropriate degrees of randomness and point separation is to cut a spherical region out of a "glass," or periodic box, that is randomly populated with particles. Another way is to stack individual shells of particles concentrically, building up the star layer by layer.

Pakmor et al. (2012) coupled the stacking technique with surface distributions generated via the HEALPix tessellation algorithm (Górski et al. 2005). HEALPix works by subdividing the surface of a sphere into  $n_p$  quadrilateral regions, or cells, of equal area and placing exactly one particle in each cell. The strength of this distribution method is that it provides both smooth and random ICs and thus minimizes the emergence of nonphysical artifacts during the system's evolution (Mohamed 2009). Another benefit to this technique is that HEALPix uses only the desired number of particles or, equivalently, cells to generate the appropriate set of (x, y, z) particle coordinates. However, the tessellation requires that particle numbers  $n_p$  satisfy the condition  $n_p = 12N^2$ , with  $N = 2^x$  for some integer x, thus considerably limiting flexibility in particle numbers.

Despite this limitation, we replicate Pakmor et al.'s (2012) concentric stacking method and use of the HEALPix algorithm to construct shellular surface particle distributions in <sup>1D</sup>MESA2HYDRO<sup>3D</sup>. HEALPix is integrated with our package via healpy (Górski et al. 2005), a Python interface to the algorithm that installs automatically with <sup>1D</sup>MESA2HYDRO<sup>3D</sup>.

Figure 1 shows a shellular particle distribution and the tessellation from which it is derived for  $n_p = 3072$  (equivalently, N = 16). All regions in the lower panel have equal area and host exactly one particle each. Particles in the upper panel are coded so that each particle has the same color as its host region below, where particles and regions are connected by the assignment of an integer 1–3072 (i.e., cell 1, in bright yellow in the lower panel, hosts particle 1, bright yellow in the upper panel, and so forth).

Both Pakmor et al. (2012) and Ohlmann et al. (2017) used stacking methods to build their models, but the former constructed density distributions that place single SPH particles in equal-volume cells. This geometric constraint requires every particle to exist in a space of size  $(r_u - r_l)^3$ , meaning that Pakmor et al.'s (2012) placement radii are determined by the equality of surface cell size and shell separation—two independent functions of the width  $r_u - r_l$ . While this equal-volume approach gives good uniformity and convergence, it allows little freedom in specifying

the locations of shells relative to each other. While this is perfectly appropriate when modeling high-density stars such as white dwarfs, it does not generalize easily to other cases. Hence, we avoid using this cubical volume constraint.

Ohlmann et al.'s (2017) method, on the other hand, allows for the free variation of shell width. It is necessary to let the radial separation of shells vary if one wishes to maintain a constant mass or number of particles per shell. This approach results in less uniform distributions than the cubical volume approach, but it is more flexible and thus more appropriate for a tool that aims to be effective for a wide variety of model stars. In our method, the relative spacing among HEALPix shells widths of slices  $r_{u,k} - r_{l,k}$ —is determined by the bounds on the mass integral  $m_{\text{shell}}$ . In the case of fixed particle mass  $m_p$ , constant mass translates to a constant number of particles per shell,  $n_p = 12N^2$ .

As central stellar densities can be several orders of magnitude larger than the local densities in the outer layers of the star, the number of equal-mass particles required to accurately represent the physical density gradients can quickly become intractable. Ohlmann et al. (2017) used some percentage of MESA's total density profile in their constructions, electing to build a particle distribution that represents only the outer layers of the star. They represented the rest of the interior by a single particle, or "core," whose mass is equal to the mass represented in the distribution subtracted from the total stellar mass. They joined these components gravitationally using a modified polytrope. While approximate, this technique preserves the region of the star that is involved in dynamical behaviors, such as mass transfer and atmospheric pulses, while limiting the scales for giant stars in a reasonable way. It also provides an effective alternative to dealing with enormous numbers of particles. Core-cutting also allows one to capture the majority the star by radius while only dealing with a small fraction of the mass.

We implement a similar method in <sup>1D</sup>MESA2HYDRO<sup>3D</sup>, allowing the user to specify the size of the extracted core either by radius or by mass. However, we offer an important caveat: while <sup>1D</sup>MESA2HYDRO<sup>3D</sup>'s core-cutting technique will always produce a particle distribution that sufficiently resembles the initial 1D density profile structurally, the situation is more complicated in 3D. In order for this to work in a smoothed particle simulation, the hydrodynamics code must be able to deal intelligently with interactions between the core mass and the rest of the particles. For this reason, <sup>1D</sup>MESA2HYDRO<sup>3D</sup> classifies the core mass as a "sink" particle distinct from the rest when writing hydrodynamic ICs.

We use the terms "depth" or "depth cut" and parameters  $m_{depth}$ ,  $r_{depth}$  to refer to the percentage of the star in total mass or radius, respectively, to which the density profile is fit. For example, rendering a model with  $m_{depth} = 5\%$  means fitting the radial extent of the star that contains the outermost 5% of the mass. We note that these depths will often correspond to regions much deeper than the physical definition of a stellar atmosphere, but we sometimes use the term "atmosphere" in this context to emphasize that penetration percentages are defined with respect to the stellar surface. The top panel of Figure 2 highlights a region corresponding to a 5% depth cut by mass in the context of a MESA density profile representing an AGB star.

Ohlmann et al. (2017) used atmospheric radial depths ranging from 0.90 to 0.98 in their models. To compare our



**Figure 1.** Top: sample particle distribution given by HEALPix for an arbitrary shell *k*. This shows 3072 particles, corresponding to N = 16. Bottom: hierarchical equal-area isolatitude pixelization of a spherical surface for N = 16, generated with *healpy*. Particles in the upper panel are color-coded according to their host regions in the lower panel. The color bar represents the particle index, which is an integer assigned to each region/particle.

models self-consistently, we fix the penetration depth to a constant percentage by radius,  $r_{depth} = 0.75 M_{\star}$ , in our 1D validation. This corresponds to mass depths between 0.5% and 7% for all of our model stars.

#### 4. Algorithm

Input data and run-time parameters are read by <sup>1D</sup>MESA2HYDRO<sup>3D</sup> from text files organized into keyword, value pairs. These are called "configuration files" and use a ".cfg" extension. The format of a configuration file follows the convention of a Fortran namelist, as is commonly used in other stellar modeling packages.

The algorithm for computing a set of shell radii proceeds as follows.

- 1. A discrete density profile r,  $\rho(r)$  corresponding to some percentage of the mass or radial distribution (as specified by the user) is extracted from a smooth MESA profile or similarly formatted file. The region representing the core mass is separated from the region to be rendered as SPH particles. These sections are shown in black and blue, respectively, in the top panel of Figure 2.
- 2. At the base of the atmosphere, we search for a solution to the equality

$$m_{\rm shell} = \int_{r_l}^{r_u} 4\pi r^2 \rho(r) \, dr = (12N^2)m_p \tag{1}$$

by shifting the upper bound on the mass shell integral,  $r_{u,0}$ , surfaceward from its local position until the integrated

mass and mass from the summation of HEALPix particles are equal to within some user-defined tolerance,  $\delta_{TOL}$ . The bottom panel of Figure 2 demonstrates the selection of an upper radius.

In Equation (1),  $m_p$  is the mass per particle and N is the HEALPix integer, both of which are set by the user. The choice of  $m_p$  and  $\delta_{\text{TOL}}$  have the largest effect on the computation time: higher values of  $m_p$  translate to less frequent solutions and hence a lower resolution profile and shorter computation times, whereas lower values of  $\delta_{\text{TOL}}$ correspond to increased precision on the location of  $r_u$  and thus longer computation times. The default tolerance is  $\delta_{\text{TOL}} = 0.01$ . The parameter combinations used for our test models are provided in Table 2.

3. When one instance of Equation (1) is satisfied, the coordinates *N* and  $r_{mid} = (r_u + r_l)/2$  are recorded in a standard text file with the prefix "NR." For other physical quantities, such as internal energy *E* or temperature log *T*, <sup>1D</sup>MESA2HYDRO<sup>3D</sup> searches the MESA data directly for the *r* values bordering  $r_{mid}$  and linearly interpolates between them to produce approximate values for  $E(r_{mid})$ , log  $T(r_{mid})$ , etc. as desired.

Following the computation of one such  $r_u$ , the subsequent lower bound  $r_{l,1}$  is set to  $r_{u,0}$ , and the process repeats until  $r_{l,1}$ ,  $r_{u,1}$  again satisfy Equation (1).

- 4. The calculation of placement radii  $r_{\rm mid}$  continues until <sup>1D</sup>MESA2HYDRO<sup>3D</sup> has subdivided the profile into k regions of variable size  $(r_u r_l)_j$ , where j = 1, ..., k. Each region j is then uniquely characterized by its N, R coordinate pair. The generation of an NR file can take anywhere from several minutes to several hours, depending on the choice of  $m_p$ ,  $\delta_{\rm TOL}$ , and the penetration depth. The completed NR file is then passed to HEALPix via healpy.
- 5. For each shell k, HEALPix distributes  $n_{p,k}$  particles across the surface of a sphere with radius  $R_k = r_{\text{mid},k}$  using the equal-cell method described in Section 3. The conversion between an NR file and an SPH-compatible IC file takes only a few seconds for particle numbers less than 10<sup>6</sup>.
- 6. Having obtained  $12N^2$  sets of (x, y, z) coordinates for the associated particles, the shells are stacked concentrically to form a 3D hollowed sphere by normalizing each HEALPix shell by its placement radius relative to the total stellar radius.
- 7. Each shell is arbitrarily rotated with respect to its neighbors in order to avoid ordered particle alignments. The rotated coordinates  $(x', y', z')_k$  are computed via the multiplication of  $(x, y, z)_k$  by the unit matrices

$$\begin{bmatrix} x'\\ y'\\ z' \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0\\ 0 & \cos\theta & -\sin\theta\\ 0 & \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\phi & 0 & \sin\phi\\ 0 & 1 & 0\\ -\sin\phi & 0 & \cos\phi \end{bmatrix}$$
$$\times \begin{bmatrix} \cos\psi & -\sin\psi & 0\\ \sin\psi & \cos\psi & 0\\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x\\ y\\ z \end{bmatrix},$$

with  $\theta$ ,  $\phi$  and  $\psi$  pseudo-randomly generated over the interval [0,  $2\pi$ ]. The pseudo-random number generator used is Python's random.random, a wrapper for the Mersenne Twister algorithm (Matsumoto & Nishimura 1998), which uses the current timestamp as a seed. New values of  $\theta$ ,  $\phi$ , and  $\psi$  are computed for every *k* but not for



**Figure 2.** Top: complete MESA density profile, from core to surface, representing the AGB phase of a  $1.8 M_{\odot}$  model star. The outer 5% of the star, by mass, is highlighted in blue. Bottom: the region we model, isolated in blue in the previous panel. The solid purple vertical line indicates a potential lower integration bound  $r_{l}$ , and the three vertical dashed lines indicate trial values of  $r_{u}$ , which is pushed rightward or toward the surface iteratively until the bounded region satisfies the mass integral in Equation (1).

every particle; otherwise, the distribution provided by HEALPix would not be preserved directly.

- 8. The final set of *k* stacked, rotated, concentric sets of (x, y, z) coordinates and the MESA attributes assigned to them particle by particle are output to a file with the prefix "IC." These arrays can be passed to subroutines that directly organize the data into file structures compatible with various hydrodynamics codes. Currently, <sup>1D</sup>MESA2HYDRO<sup>3D</sup> supports output in the GADGET-2 unstructured binary and hdf5 formats, the Phantom binary format, and a simple ASCII text file. The user may control the precision with which the numerical data are written to the IC file, as well as the format of that file, using flags in the configuration file. For example, filetype=phantom\_binary will produce a binary file in the Phantom format.
- 9. Using binning parameters specified by the user,  ${}^{1D}$ MESA2HYDRO ${}^{3D}$  can reload the 3D data it has generated directly and reduce them to a 1D *r*,  $\rho(r)$  curve. The package does not use a smoothing kernel or any other SPH features. To verify compatibility with a particular SPH code, the user should apply the smoothing kernel used in that code to the output distribution or use a tool such as SPLASH (Price 2007, 2012).

The integral in Equation (1) is solved using a fourth-order Runge–Kutta scheme with adaptive step-size refinement (Runge 1895). This method was found to be more well suited to our problem than, for example, Python's scipy.integrate function due to the large variation in radial width that can correspond to a fixed shell mass. One can provide an initial guess for the integration step size in the configuration file, though this will be adjusted automatically as necessary depending on the local shape of the density profile and the particle mass and solution tolerance provided by the user. An inappropriate choice in step size may prolong the first few shell calculations, but it will not have a large impact on the computation time. Changes in the solution tolerance, however, scale linearly with computation time.

The <sup>1D</sup>MESA2HYDRO<sup>3D</sup> workflow is subdivided into two main procedures: the first translates a 1D density profile to an NR file by calculating the shell placement radii, and the second translates an NR file to an IC file using the radial spacings and HEALPix tessellation. As the former conversion takes much longer than the latter, the subroutines are written to be executable in isolation. Within these subroutines, many other components of the workflow can be isolated by manipulating the appropriate flags in a configuration file.

### 5. Software Package

The package <sup>1D</sup>MESA2HYDRO<sup>3D</sup> is written in Python and it interfaces with various C and Fortran libraries needed by HEALPix, HDF5, Phantom, SPLASH, and (optionally) the MESA code itself. The test suite is verified using data generated with MESA version 10398 and Phantom (2019), so the interfaces are guaranteed to be compatible with these versions of the external software.

Several nonstandard Python packages are required by <sup>1D</sup>MESA2HYDRO<sup>3D</sup>: cython h5py, hdf5lib, healpy, matplotlib.pyplot, numpy, and random. The main workflow is not currently parallelized, but it is thread safe so long as the user does not direct the output of two NR calculations to the same file.

Our package does not require MESA itself or a hydrodynamics code to run, though it must receive the 1D profile in a format that uses MESA-style keywords as column headers.

One can freely obtain <sup>1D</sup>MESA2HYDRO<sup>3D</sup> by contacting the authors and install it via the standard Python setup procedure. Upon public release, it will be available from GitHub https://github.com/mjoyceGR/MESA2HYDRO or via Python's pip tool. Detailed installation and setup instructions are provided in the user's guide, also available on GitHub.

The user can specify  $\sim 20$  parameters in a <sup>1D</sup>MESA2HYDRO<sup>3D</sup> configuration file. These include operational attributes (e.g., file names), physical parameters (e.g., particle mass), numerical specifications (e.g., step size for the numerical integrator), and plotting controls for the recovery test routines (e.g., bin number). These parameters may also be specified as command line arguments. Default values are set for all user controls and correspond to a solar-like model star that uses pre-generated MESA data. The program reverts to these values only if neither a configuration file nor any command line argument is specified. A sample configuration file with parameters corresponding to each of the test cases presented here is provided in the <sup>1D</sup>MESA2HYDRO<sup>3D</sup> suite.

The operation cycle of <sup>1D</sup>MESA2HYDRO<sup>3D</sup> proceeds as shown in Figure 3. The 1D input data are processed by routines



Figure 3. Flow of control diagram for <sup>1D</sup>MESA2HYDRO<sup>3D</sup>.

in the MESA handling library. The data are reduced to a set of k coordinates N, R via methods contained in the numerical routines module, from which HEALPix then generates the requisite set of (x, y, z) coordinates. The complete set of particle positions is written to a file whose format is specified by the user via the input-output (I/O) module. By default, <sup>1D</sup>MESA2HYDRO<sup>3D</sup> writes ASCII text files, but this can result in cumbersome file sizes for large particle numbers. Using flags in the configuration files,  $^{\rm 1D} \rm MESA2HYDRO^{3D}$  can produce output in the specific binary formats required by various SPH codes. Some of these require the HDF5, or hierarchical data format, file format, which is used to organize large data files for supercomputing. The fidelity of <sup>1D</sup>MESA2HYDRO<sup>3D</sup>'s distribution to the initial density profile can then be assessed optionally using the package controls; the user may reload the 3D distribution, compress it to a 1D radial curve, and display this against the data loaded from MESA. The most common sources of discrepancy between the input density profile and the output distribution are insufficient tolerance on the integral solution and low resolution imposed by the use of heavy particles.

A full execution of this cycle may take anywhere from several minutes to a few hours on one thread, depending primarily on the atmospheric depth and the tolerance on Equation (1). Generating the NR file is the largest source of computation time—typically on the order of minutes to hours. Generating an IC from the NR file does not take longer than several seconds for reasonable particle numbers. Exact run times and other computational aspects for the test suite are given in Table 2.

In Figure 3, dark blue square boxes show components that are the original work of the authors. These can be manipulated directly by the user via the configuration file. Components represented by green ovals are external software incorporated into <sup>1D</sup>MESA2HYDRO<sup>3D</sup>, where interfaces are also the original work of the authors. Components represented by red ovals are base programs; for example, MESA and Phantom. These can be substituted for any similar SSEC or SPH code, respectively. Each of these components, as well as all critical subroutines included with <sup>1D</sup>MESA2HYDRO<sup>3D</sup>, are described thoroughly in the user's guide.

In addition to the main program, the <sup>1D</sup>MESA2HYDRO<sup>3D</sup> package contains a few basic tools. These include a script for confirming that a MESA profile is reasonable and a guide for selecting appropriate values for particle mass and initial step size, among others (see the user's guide for more detail on additional features).

#### 6. Validation

Two situations of particular interest in stellar hydrodynamics are (1) pulsation and instability and (2) dynamical interactions. The latter often involves mass exchange between a radially extended, evolved star and a compact companion, such as a white dwarf. Such stars will necessarily have very different outer density structures, so <sup>1D</sup>MESA2HYDRO<sup>3D</sup> must be able to generate ICs for stars encompassing a broad spectrum of physical properties. To demonstrate this capability, we test <sup>1D</sup>MESA2HYDRO<sup>3D</sup> on five stellar models that span a range of masses, evolutionary phases, and internal physical configurations.

We note that the radial extent captured by a given mass depth can vary dramatically depending on the star's density structure; for example, the outermost 30% of a star by radius contains 5% of the mass of a  $1 M_{\odot}$  main-sequence star but less than 0.1% of the mass of a  $90 M_{\odot}$  supergiant. To compare our results systematically, the radial depth is fixed across the set of sample models presented for demonstration, and hence the depth by mass varies among them.

Smooth, physically realistic density profiles are produced with the MESA inlists included in this package. Unless otherwise specified, the 1D models are generated using the MESA equation of state, the Grevesse & Sauval (1998) opacities, and the "basic.net" nuclear reaction network. Since metallicity is known to impact stellar atmospheres (Thoul et al. 2003; Porto de Mello et al. 2008; Asplund et al. 2009, and many others), we also maintain approximately solar abundance (Z = 0.02) in each star. Choices for additional parameters (convective overshoot values, additional nuclear reaction rates, etc.) can be found in the inlists directly. Our choices for the fundamental astrophysical attributes of each test model are discussed below.

#### 6.1. Test Cases

**Model 1:** solar-like main-sequence star. This is a standard model with solar mass  $(1.0 M_{\odot})$  and metallicity (Z = 0.02) that terminates 5 Gyr after collapse onto the zero-age main sequence. The age, initial and final masses, metal abundance,

 Table 1

 Summary of Physical Properties of Modeled Stars

Туре	$M_{ m i}$	$Z_{i}$	Age	$M_{ m f}$	R	$\log L$	$T_{\rm eff}$	Stop Condition	Pre-built Model?
Main sequence	1.0	0.02	5.0	1.0	1.0	0.0	5760	$max_age = 3.0d9$	no
Red giant	1.0	0.02	12.0	1.0	3.44	0.76	4820	$max_age = 12.0d9$	no
Red supergiant	90	0.02	0.00015	90	9.29	6.14	65100	H-burning limit	no
TP-AGB	2.55	0.02	0.77	2.54	125	3.28	3400	$stop_at_TP = True$	no
White dwarf	1.0	0.02	>15	1.3	0.004	-0.48	68400	Nuclear-burning limit	yes

Note. Basic physical attributes of the test models. Masses are in  $M_{\odot}$ . Here Z is the dimensionless mass fraction of metals. Ages are in Gyr. Radii are in units of  $R_{\odot}$ . Log L are in units of log  $L/L_{\odot}$ . Effective temperatures are in K. Stopping criteria are used to halt the evolution of the model at the correct phase. The first two models are stopped at certain ages corresponding to the correct evolutionary phase. Models 3 and 5 are stopped according to limits on their nuclear reactions, which indicate the correct evolutionary phases. Model 4 uses a flag specifically for stopping evolution during a thermal pulse.

radius, luminosity, and temperature are given for this and subsequent models in Table 1. The profile roughly reflects the interior structure of the Sun. Solar-mass stars transport energy via convection in their outer layers and radiation in their cores. Though the Sun at its current age is not especially dynamic, interactions with the convective envelope produce mixing events in the later stages of a star's life, which can lead to instability. This, and the fact that the Sun is used as a calibrator for 1D stellar models, make this a particularly important test case (Joyce & Chaboyer 2015, 2018a, 2018b). *Model 2:* solar-like red giant. This model has a mass of  $1 M_{\odot}$ and solar metallicity. It terminates at 12 Gyr, after it has left the main sequence and ascended onto the red giant branch. Red giants of roughly this mass and age are common in stellar populations such as globular clusters, and they frequently appear in multi-star systems. This model is a useful template for the canonical red giant in a binary system. Model 3: supergiant. This model has an initial mass of  $90 M_{\odot}$  and solar metallicity and terminates in the middle of its red giant phase. Because of its mass, the interior physics and subsurface density structure differ considerably from those of model 2. At its termination, the interior will have a similar configuration in terms of convective versus radiative zones, but this model contains nested hydrogen-, helium-, carbon-, and oxygen-burning regions. Most importantly, the outer layers of this star are highly radially extended. While the outermost 5% of the mass is contained within the outermost 20% of the radius for a solar-like red giant, the same radial proportion holds less than 0.5% of the mass in this case. This model is guided by the inlist used to generate Figure 44 in Paxton et al. (2015), and our parameter choices are informed by those of the "90M\_logT\_9.35.mod" model in the high-mass test suite of MESA version 8118. We include the inlist adapted for mesa-r10398 with <sup>1D</sup>MESA2HYDRO<sup>3D</sup>. Model 4: TP-AGB star. This model has an initial mass of 2.55  $M_{\odot}$  and metallicity Z = 0.01. It terminates after the third dredge-up (3DU) during the late thermal pulse phase along the AGB. At this point in its evolution, the star's pulsations have caused a small amount of mass loss, so the initial mass is slightly higher than the mass integrated in its density profile. This model adopts the opacities based on Asplund et al. (2009) and the "Mesa\_49.net" nuclear reaction grid.

The metallicity, opacity prescription, and nuclear network deviate from what is used in other models because this inlist is based on an experimental inlist designed specifically to achieve good convergence on post-3DU thermal pulses; this is a notoriously difficult evolutionary phase to model correctly (see, for example, Molnár et al. 2019). It also borrows overshoot and mixing prescriptions from inlists for TP-AGB models published by Tashibu et al. (2017) and invokes other suggestions from the MESA collaboration directly (see the inlist and Paxton et al. 2015 for more detail). Model 5: white dwarf. This is a solar-mass white dwarf, and it is the only one in our suite that uses a pre-built MESA model. Specifically, we use wd3\_1Msolar.mod, one of several white dwarf models included with MESA version 10398. The parameter specifications required to produce a reasonable profile for the outer layers of a white dwarf are very different from those of the previous models due to the fundamental difference between white dwarfs and the outer regions of "living" stars, namely, the equation of state. A nondifferentiable region may emerge due to the disruption in the stellar profile where the equations of state governing different regions, e.g., cores versus atmospheres, meet, or it may be the consequence of perfectly physical discontinuities in the chemical composition of the star. For a star undergoing active nuclear fusion, such discontinuities emerge deep in the interior and would not affect our modeling of the outer layers. For a white dwarf, however, discontinuities occur very near the surface, as white dwarfs have inert cores under incredibly thin atmospheres. This model includes Type 2 opacities and invokes the "co\_burn.net" nuclear reaction network, which accounts for additional carbon/oxygen burning. This model also includes an accretion rate of  $10^{-9} M_{\odot} \text{ yr}^{-1}$ during the white dwarf phase, which accounts for the small increase in mass over its initial solar value. A (non-MESA) stellar structure model provided by Maurizio Salaris (Cassisi et al. 2006; Salaris et al. 2013) was used to guide additional parameter selections for this model.

Table 1 summarizes basic physical attributes of the models, including their stopping criteria. This set is by no means exhaustive but does cover key regions of the H–R diagram and includes types of stars that are commonly modeled in hydrodynamics simulations.

#### 6.2. Validation: MESA to Particle Comparison

We quantify the consistency between the MESA-generated source density profiles and the density profiles estimated from particle distributions recovered from <sup>1D</sup>MESA2HYDRO<sup>3D</sup>. Figures 4–8 contain the following.

(1) In the top panels, semi-log density profiles of the MESAgenerated source and particle data are shown in physical units. A density distribution is estimated from the particle



**Figure 4.** (Top) Physical density profile  $\rho(r)$  pulled from the input stellar structure model against an approximate 1D density reconstruction from the reloaded particle data. (Middle) Inverted cumulative mass distributions for the input and output data. (Bottom) Residuals between fits to the cumulative mass distributions as a function of radius for a solar-like model.

data using bin numbers ranging from 20 to 30 among the test cases.

(2) In the middle panels, normalized cumulative mass distributions for source and particle data are shown. They are inverted to reflect the curvature of the (unlogged) density profiles and normalized to remove the dependence on particle mass. We use  $m_p = 10^{-7}$  in all cases but the supergiant, which uses  $m_p = 10^{-6}$ , but this is an arbitrary choice and does not impact the shape of the density and mass distributions. A third-degree polynomial

$$\rho_f(r) = Ar^3 + Br^2 + Cr + D \tag{2}$$

is applied to each curve to allow for comparison between  $\rho(r)$  predicted by each distribution.

(3) The bottom panels present residuals in terms of percent error,  $100 \times |\rho_f(r) - \rho_g(r)|$ , as a function of radius,

where  $\rho_f(r)$  is a fit of Equation (2) to the source density profile and  $\rho_e(r)$  is the binned particle data.

(4) The error is also given as a single rms score in the bottom panels,

$$\sigma_{\rm rms} = \sqrt{\Sigma_k^N \frac{(\rho_f(r) - \rho_g(r))^2}{N_{\rm shells}}},$$
(3)

calculated only over the radial extent shown.

We generate sets of models mapping the outer 25%, 50%, and entire star by radius ( $r_{depth} = 0.75$ , 0.5, and 0.0 in the convention of the configuration files). Figures 4–8 show results for  $r_{depth}$  fixed to  $0.75R_{\star}$  and  $\delta_{TOL} = 0.01$ . We fix the HEALPix integer to N = 8 in each case but allow  $m_p$  to vary among models. These demonstrate the goodness of recovery for models of varying structure, spanning 18 dex in density, constrained by computation times on the order of hours and tractable particle numbers (<0.5 million). Table 2 shows the numbers of shells and particles needed to generate Figures 4–8, the radial and mass percentages modeled in each case, the computation times, and the rms measure of goodness of fit.

The maximal discrepancy between input and output density profiles with these parameter settings is less than roughly 10% for all models and less than 5% for all but the TP-AGB star. The rms error for the TP-AGB star is more than double the next-most-discrepant model, the white dwarf, whose rms error is itself more than double that of the other three test models. One factor contributing to these differences in agreement is the comparatively larger range of densities encompassed in the outer 25% of the AGB star and white dwarf—about 2.2 dex versus 1.4 dex for the main-sequence star, red giant, and supergiant.

As shown in Figure 7, <sup>1D</sup>MESA2HYDRO<sup>3D</sup> struggles most with resolving the outermost portion of the stellar atmosphere, which is unsurprising given the sparseness of this region. If one's primary goal is to preserve the structure of the outer layers with high fidelity, a smaller particle mass and shallower  $r_{depth}$  would be more appropriate choices than those used in Table 2.

We note that some subtleties, such as the hook in the AGB star's outermost density profile in the top panel of Figure 7, may be lost at the expense of large choices for  $m_p/$ lower particle numbers/faster integration times. Greater consistency between the input and <sup>1D</sup>MESA2HYDRO<sup>3D</sup>-rendered density profiles is always achievable with larger particle numbers and longer computation times, but distributions with extremely large particle counts will be intractable for the user, as well as for most hydrodynamics codes. There is also a point of diminishing returns when balancing computation time against reduction in  $\sigma_{\rm rms}$ , and it is up to the user to decide which parameters are appropriate for his/ her/ their problems. Those presented here serve only as a guide.

In addition to the tests summarized in Table 2, we generate distributions over the same radial span with equivalent parameter values using a weaker tolerance,  $\delta_{\text{TOL}} = 0.05$ , and note the difference in computation time. For the main-sequence model, the execution takes 0.16 hr at  $\delta_{\text{TOL}} = 0.05$  versus 0.74 hr at  $\delta_{\text{TOL}} = 0.01$ . For the red giant, the run time drops to 0.99 hr; for the supergiant, AGB star, and white dwarf, the run times drop to 1.31, 0.73, and 1.22 hr, respectively, from the times given in Table 2. The corresponding loss in fidelity for such shallow radial penetration depths is high, but increasing



Figure 5. Same as Figure 4 but for a solar-type red giant model.



Figure 6. Same as Figure 4 but for a red supergiant.

 $\delta_{\text{TOL}}$  when integrating half or all of the radial profile has a less significant impact on the overall shape of the recovered density profile. The diminished resolution will impact low-density regions most. In the case where one is interested in the density structure of the entire star rather than strictly the outer layers, this loss may be worth the decrease in computation time.

We can understand the impact of the choice in particle mass on computation time by comparing the run-time values in Table 2 to those of the modified models used to generate the test ICs for verification with Phantom (these tests are discussed in more detail in Section 6.3). Using  $\delta_{\text{TOL}} = 0.01$  and particle masses of  $10^{-5} M_{\odot}$  for the main-sequence star, red giant, and white dwarf and  $10^{-4} M_{\odot}$  for the AGB star and supergiant, <sup>1D</sup>MESA2HYDRO<sup>3D</sup>'s search for radial solutions to Equation (1) over the majority of the stellar profile ( $r_{\text{depth}} \rightarrow 0$ ) takes  $\leq 2$  hr for each model. Calculation times for the red supergiant and white dwarf are longest, whereas the NR coordinates for the mainsequence star, red giant, and AGB star take less than 40 minutes to generate.

We find that, so long as the integration tolerance is maintained, choosing higher values of  $m_p$  generously improves

the speed of the NR routine without heavily impacting the shape of the damped density profile at the end of a simulation with Phantom. We find that precision on the location of the shell radii is more important for preserving agreement with the initial MESA profile than resolution in particle mass, so it is preferable to lower  $\delta_{\text{TOL}}$  rather than  $m_p$  when seeking improvements in fidelity without huge increases in computation time. We note, however, that these are appropriate trade-offs only for distributions that encompass most of the star by radius.

# 6.3. Validation: 3D Verification

A cross section of a <sup>1D</sup>MESA2HYDRO<sup>3D</sup>-generated particle distribution for the TP-AGB model is shown for demonstration in Figure 9, and the 3D distribution is shown in Figure 10. The bottom panel of Figure 10 invokes a smoothing kernel. Distributions for all test models look similar when viewed with an SPH-compatible program (Helly 2003; Price 2007).

We further analyze each of the five test distributions using the Phantom SPH code (Price et al. 2018). It is easiest to achieve stable distributions in Phantom as  $r_{depth}$  approaches



Figure 7. Same as Figure 4 but for a TP-AGB model.

zero, but the resulting particle numbers for the same combinations of  $m_p$  and  $\delta_{\text{TOL}}$  given in Table 2 exceed 10 million for some models (e.g., the white dwarf). While it is possible to calculate the evolution of 10 million particles with Phantom, the computing times extend into weeks. As rigorous hydrodynamical analysis is beyond the scope of this paper, we perform the 3D tests using lower-resolution versions of the models presented in Table 2. With the exception of larger values of  $m_p$  and penetration depths approaching zero, all parameters of the ICs run with Phantom are equivalent.

We evolve the distributions for 10 dynamical timescales  $(\tau_{dyn})$ , following the damping prescription of Ohlmann et al.'s (2017) Equation (9), implemented in Phantom by Reichardt (2019):

$$\tau(t) = \begin{cases} \tau_{\rm l}, & t < 2t_{\rm dyn} \\ \tau_{\rm l} \left(\frac{\tau_2}{\tau_{\rm l}}\right)^{\frac{t-2t_{\rm dyn}}{3t_{\rm dyn}}}, & 2t_{\rm dyn} < t < 5t_{\rm dyn} \\ \infty, & t > 5t_{\rm dyn}. \end{cases}$$
(4)



Figure 8. Same as Figure 4 but for a white dwarf model.

Dynamical timescales are proportional to density and thus vary among the models. Very rough estimates are given by

$$t_{\text{freefall}} \approx \frac{2100}{\sqrt{
ho}},$$

where the numerator is in seconds and the denominator is in  $g \,\mathrm{cm}^{-3}$ . The order of  $t_{\rm dyn}$  for each model is estimated from  $\rho_{\star} \sim \frac{M_{\star}}{R_{\star}^3}$  and given in Table 3.

We consider the ICs to be valid as long as a few conditions are satisfied. First, all physical attributes assigned via <sup>1D</sup>MESA2HYDRO<sup>3D</sup> must be read and correctly understood by Phantom. Second, the shape of the density profile must be preserved at  $t = 10t_{dyn}$ . Last, if the velocity dispersion is small after evolution without damping for  $5t_{dyn}$ , we consider the final configuration to be in hydrostatic equilibrium. However, we do not make this a strict criterion for claiming consistency, as there may be valid physical reasons for instability after several dynamical timescales for some of our models.

The relationship between (1) the initial MESA profile, (2) the 1D approximation to the particle distribution generated with



Figure 9. Sample (every 200th particle of the array of ~460,000) of the x (pink), y (green), and z (blue) components from a particle distribution representing the TP-AGB model shown against radial coordinate  $r = \sqrt{x^2 + y^2 + z^2}$ . The vertical dashed line indicates the innermost radius that was captured by the TP-AGB model's depth cut of 1%. This slice corresponds to Figure 7.

 Table 2

 <sup>1D</sup>MESA2HYDRO<sup>3D</sup> Run-time Parameters and Goodness of Recovery for Test Models

Star	Ν	$m_p$	R <sub>*</sub>	M <sub>*</sub>	$\Delta_{r,\text{initial}}$	N <sub>shells</sub>	n <sub>p</sub>	tgen	$\sigma_{\rm rms}$
Standard solar	8	$1 \times 10^{-7}$	0.75	0.0167	$1.00 \times 10^{8}$	441	338,688	1.311	0.018
Solar red giant	8	$1 \times 10^{-7}$	0.75	0.0650	$1.00 \times 10^{8}$	852	654,336	4.039	0.022
Red supergiant	8	$1 \times 10^{-6}$	0.75	0.0034	$1.00 \times 10^{11}$	453	347,904	6.671	0.020
TP-AGB	8	$5 \times 10^{-7}$	0.75	0.0449	$1.00 \times 10^{10}$	298	228,864	6.652	0.118
White dwarf	8	$1 \times 10^{-7}$	0.75	0.0330	$1.00 \times 10^{5}$	556	427,008	5.128	0.045

Note. Computational and physical features of each test model are shown for  $r_{depth} = 0.75R_{\star}$  and  $\delta_{TOL} = 0.01$ , corresponding to Figures 4–8. Particle masses are in units of  $M_{\odot}$ , and N is the HEALPix integer. Initial step sizes are in physical units (cm), and  $t_{gen}$  is the generation time for the NR coordinates in hours. Generation times for IC files are negligible, typically on the order of 5–10 s.

<sup>1D</sup>MESA2HYDRO<sup>3D</sup>, (3) the <sup>1D</sup>MESA2HYDRO<sup>3D</sup> output reloaded from Phantom ( $t_{dyn} = 0$ ), and (4) the converged particle distribution at  $10t_{dyn}$  for the main-sequence test model is shown in Figure 11. By visual estimation, there is excellent agreement among all four density profiles in 1D.

We note that some flattening of the profile occurs between Phantom's interpretation of the <sup>1D</sup>MESA2HYDRO<sup>3D</sup> particle distribution and between  $0t_{dyn}$  and  $10t_{dyn}$ , and that the inner and outer boundaries of the star are less well resolved than the central region. The difference between the raw output from <sup>1D</sup>MESA2HYDRO<sup>3D</sup> and the distribution reloaded from Phantom at t = 0 is that, in the former case, the output from <sup>1D</sup>MESA2HYDRO<sup>3D</sup> is converted back to radial coordinates and assigned the nearest density from the MESA profile directly. In the latter, the density values assigned to each particle reflect Phantom's own calculations based on nearest neighbors using a smoothing kernel.

Appropriate smoothing lengths for the gas particles are computed in  $^{\rm 1D} \rm MESA2HYDRO^{\rm 3D}$  according to

$$h_i = 1.2 \times (m_p/\rho_i)^{1/3},$$

where *i* is the index in MESA of the radius corresponding to the particle's shell radius, and  $\rho_i$  is the corresponding MESA density value.

As one can see in Figure 11, there is a spread among the yellow particles, reflecting variations in density estimates for particles situated on the same shell. While these fluctuations quickly dissipate during the damping procedure, they can also be initially mitigated by increasing the precision on Equation (1) (i.e., lowering  $\delta_{\text{TOL}}$  and/or  $m_p$ ) when generating the NR file.

Figure 12 shows XY cross sections of the 3D particle distributions corresponding to the  $t = 0t_{dyn}$  and  $10t_{dyn}$  curves in Figure 11. Here we see that the distribution at  $10t_{dyn}$  has settled into a configuration that appears more random and slightly less radially extended. In reality, some flattening of the density profile and radial extension occurs for all models in the 3D simulations.

Figure 12 also shows a small black region in the center of the density field in the t = 0 distribution—suggesting a central density of zero, which is subsequently replaced by a value close to the true stellar central density at t = 10. In Phantom, the core mass is modeled as a sink particle that interacts only

		Paran	neters for MESA2H	I I DRO Distribution	ns Tested with Phanton	n	
Star	$m_p$	$N_p$	$M_{\star}$ (g)	$R_{\star}$ (cm)	$ ho_{\rm avg}~({\rm g~cm^{-3}})$	$t_{\rm dyn}$ (s)	Phantom EOS
Standard solar	$10^{-5}$	102,144	$1.98 \times 10^{33}$	$7.02 \times 10^{10}$	$1.37 \times 10^{0}$	$1.80 \times 10^{3}$	Adiabatic; $\gamma = 5/3$
Solar red giant	$10^{-5}$	102,144	$1.98 \times 10^{33}$	$2.40 \times 10^{11}$	$3.46 \times 10^{-2}$	$1.13 \times 10^4$	Adiabatic; $\gamma = 5/3$
Red supergiant	$10^{-4}$	64,512	$1.78 \times 10^{35}$	$1.18 \times 10^{14}$	$2.57 \times 10^{-8}$	$1.31 \times 10^7$	Adiabatic; $\gamma = 5/3$
TP-AGB	$10^{-5}$	193,536	$5.05 \times 10^{33}$	$8.69 \times 10^{12}$	$1.84 \times 10^{-6}$	$1.55 \times 10^{6}$	Adiabatic; $\gamma = 5/3$
White dwarf	$10^{-5}$	134,400	$1.98 \times 10^{33}$	$2.78 \times 10^{8}$	$2.20 \times 10^7$	$4.48 \times 10^{-1}$	Helmholtz

Table 3

Note. In all cases,  $\delta_{TOL} = 0.01$ . Here  $r_{depth}$  is approximately zero for all models, with the exception of the supergiant, which uses  $r_{depth} = 0.35$  due to the difficulty of resolving the extreme densities in the stellar core using a particle mass that is suitable for the rest of the layers. When  $r_{depth} = 0.0$  is used for the supergiant, the <sup>1D</sup>MESA2HYDRO<sup>3D</sup> solution time jumps from approximately 1.6 to 19 hr, and the particle number increases from  $\approx 65,000$  to more than 1 million.



**Figure 10.** Top: <sup>1D</sup>MESA2HYDRO<sup>3D</sup>-generated particle distribution, as rendered by the SPH viewer gadgetviewer, for the TP-AGB model. The region modeled extends from the central yellow ring to the exterior. The center is hollow (as demonstrated in Figure 9); particles that appear in the center are physically located at  $r \ge \sim 7.5 \times 10^{12}$  cm but displayed in the plane of the page. Bottom: same as above but with a smoothed-density projection applied. Color-coding reflects density, where yellow regions are most dense and red regions are least dense. Note that in the case of the smoothed distribution, the density coloring reflects the presence of the large point mass we have placed at the center of the star.

gravitationally with the gas particles, and the softening length  $(h_{sink})$  of the sink particle is calibrated to be half of the innermost radius of the gas shells. This is placed at the physical



**Figure 11.** For the solar-like main-sequence star, (1) the MESA profile is show as a blue line, (2) the output from <sup>1D</sup>MESA2HYDRO<sup>3D</sup> reduced to 1D is shown by green dots, (3) the distribution reloaded from Phantom at  $t = 0t_{dyn}$  is shown by yellow stars, and (4) the stable particle distribution reloaded from Phantom at  $t = 10t_{dyn}$  is shown by purple triangles.

center of the distribution. The "filling in" of the density field at the center over the simulation time is caused by Phantom's attempt to smoothly connect the fields of the gas particles and the central gravity well (for details on the mathematics of how this is achieved, see Price et al. 2018).

Even in cases where nearly all of the stellar radius is captured by <sup>1D</sup>MESA2HYDRO<sup>3D</sup>, the sink particle will exert a force on the gas particles proportional to the integrated density in the center of the star. As such, the sink particle is crucial in the balancing of forces required to achieve hydrostatic equilibrium, and the less work Phantom needs to put into smoothly connecting the pressure of gas particle, the more stable its solution will be. This is why it is helpful, in terms of computation time and accuracy on the 3D end, to set  $r_{depth}$  close to zero in <sup>1D</sup>MESA2HYDRO<sup>3D</sup>. The trade-off will be either lower fidelity in the outer layers of the star or large particle numbers; prioritizing these attributes is, once again, a matter of preference, and the best options will vary depending on the problem.

To further demonstrate that particle configurations generated with <sup>1D</sup>MESA2HYDRO<sup>3D</sup> behave reasonably in hydrodynamic simulations, we examine the evolution of the velocity distribution in the main-sequence star, a system we know should not exhibit any mass loss, radial expansion, or



**Figure 12.** For the main-sequence model, the left panels show features of the particle distribution at  $t = 0t_{dyn}$ , and the right panels show the same at  $t = 10t_{dyn}$ , in hours. Top: physical particle distribution in the cross section. Bottom: density field in the XY plane.

dynamical behavior. Figure 13 shows Mach number (velocity over local sound speed,  $c_s$ ) versus velocity for a subset of the particles in the main-sequence model at the beginning and end of its evolution with Phantom. This clearly demonstrates the trend toward smaller particle velocities, on average, with increasing evolutionary time, inclusive of evolution over five dynamical timescales without damping. The rms velocities for t = 0 and 10 are  $2.8 \times 10^6$  and  $2.1 \times 10^5$  cm s<sup>-1</sup>, respectively. Table 3 summarizes the 3D simulation parameters for each test model.

In most cases, the number of particles that become gravitationally unbound from the star (on our simulation timescale) is zero or negligible; however, the AGB model in particular is prone to mass dissipation and rapid radial expansion. This is not necessarily unphysical, as the MESA profile for this model does characterize a star in the midst of dynamical activity, and the internal energy associated with this state is propagated through <sup>1D</sup>MESA2HYDRO<sup>3D</sup> into the hydrodynamic ICs. The generation of hydrodynamically stable models of AGB stars and other radially extended giants that do not require external damping or artificial forces remains an active area of research, and this is not a problem we attempt to solve in this study. However, though rigorous assessments of the evolution of these systems are beyond the scope of this paper, we believe that <sup>1D</sup>MESA2HYDRO<sup>3D</sup> will be a valuable tool in the search for solutions to these and other outstanding problems in stellar hydrodynamics.

As a baseline assessment, we check that the shapes of the <sup>1D</sup>MESA2HYDRO<sup>3D</sup>-generated distributions remain intact over  $10t_{dyn}$  and compare the <sup>1D</sup>MESA2HYDRO<sup>3D</sup> distributions to polytropic test models (available by using the "star" Makefile option in Phantom; see Price et al. 2018) that use the same



**Figure 13.** Mach number  $v/c_s$  vs. velocity for a subsample of the particles comprising the 3D main-sequence model. A snapshot at  $t = 0t_{dyn}$  is shown by blue circles; at  $t = 10t_{dyn}$ , it is shown by orange triangles.

number of particles, maximum radius, equation of state/ adiabatic index, and central density. In all cases, the <sup>1D</sup>MESA2HYDRO<sup>3D</sup> and polytropic distributions show similar evolution over  $10t_{dyn}$ . Both undergo some radial expansion, typically on the order of 5%–20%  $R_{\star}$ . However, unlike the polytropic models, the <sup>1D</sup>MESA2HYDRO<sup>3D</sup> distributions are derived directly from MESA density profiles.

We do note that in the case of the white dwarf, there is little difference in the evolution of a <sup>1D</sup>MESA2HYDRO<sup>3D</sup> distribution versus a polytrope generated with Phantom, and it is more time-consuming to use <sup>1D</sup>MESA2HYDRO<sup>3D</sup>. It is also perhaps most appropriate to use the "whitedwarf" Makefile setup in Phantom, which involves more sophisticated nuclear reaction networks that are not yet publicly available. Our tool nonetheless renders white dwarf density profiles effectively, though other means may be more appropriate for this type of star.

#### 7. Summary and Conclusions

We have presented <sup>1D</sup>MESA2HYDRO<sup>3D</sup>, a tool for generating ICs for hydrodynamical simulations through the translation of 1D, SSEC-based density profiles to 3D particle distributions. We have presented a technique for generating *N*, *R* coordinates, modeled in part after similar efforts by Pakmor et al. (2012) and Ohlmann et al. (2017). We have explained <sup>1D</sup>MESA2HYDRO<sup>3D</sup>'s operational features, primary algorithm, and underlying numerical methods. We have verified <sup>1D</sup>MESA2HYDRO<sup>3D</sup>'s functionality on

We have verified <sup>1D</sup>MESA2HYDRO<sup>3D</sup>'s functionality on five model stars generated with MESA and discussed the physical and computational parameters used in successful runs. We have demonstrated that <sup>1D</sup>MESA2HYDRO<sup>3D</sup> can convert radial profiles to particle distributions with fidelity across 18 dex in density by applying <sup>1D</sup>MESA2HYDRO<sup>3D</sup> to stellar models that vary in structure from compact, solar-mass white dwarfs to supermassive, radially extended red giants. We have verified <sup>1D</sup>MESA2HYDRO<sup>3D</sup>'s utility as an IC-generating tool using the Phantom SPH code.

We intend for this tool to be openly distributed, freely available, and regularly maintained, and we anticipate that it will help in the search for solutions to a variety of problems in stellar astrophysics. This work was supported by Martin Asplund, the Research School of Astronomy and Astrophysics at the Australian National University, and funding from Australian Research Council grant No. DP150100250. This work was additionally supported by Brian Chaboyer and grant AST-1211384 from the American National Science Foundation.

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