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# Stellar Structure Calculation Report

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## ABSTRACT

I report a calculation of a five-solar mass ($5M_\odot$), zero-age main sequence (ZAMS) star with the elemental abundances of $(X, Y, Z) = (0.70, 0.26, 0.04)$ by numerically integrating four coupled differential equations and respecting the physically-motivated boundary conditions. The equations and the numerical methods worked as intended except for the inward integration from the surface, which posed difficulty with the automated optimization. Using the outward integration from near the center and adjusting parameters manually, I estimate the radius $R$ and luminosity $L$ to be $1.34R_\odot$ and $1.26 \times 10^3 L_\odot$, respectively.

*Keywords:*

## 1. INTRODUCTION & THE MODEL

I aim to model a five solar mass ($5M_\odot$), zero-age main sequence (ZAMS) star. The mass is chosen to study the differences from the sun, which mostly generates its energy by p-p chain. With the larger mass, higher central temperature and pressure is expected, and I expect to see more CNO cycle–based energy generation and larger fraction of the convective region(s). For a simple comparison to the sun, I choose a similar, but slightly different, elemental abundances of $(X, Y, Z) = (0.70, 0.26, 0.04)$.

The stellar structure is modeled using four coupled differential equations that characterize the radial profile of key quantities – energy generation, energy transport, equation of state, and conservation of mass.

Regarding the profile of the interior structure, I make a few key assumptions to simplify the project:

- The star is a ZAMS: the time-dependent changes in elemental abundances and its profile is ignored.
- The star is in a spherical symmetry.
- The star's chemical composition is homogeneous: i.e., elemental abundances is not a function of radial position.
- The star is made of an ideal gas, and therefore pressure is a sum of ideal gas pressure and radiation (photon) pressure.
- The star contains nearly all of its mass below photosphere.
- The star transports energy by either radiation or convection: no overshooting, no conduction.

Under the above assumptions, in the mass-shell space, the four differential equations for the four variables (luminosity $l$, pressure $p$, englosing radius $r$, and temperature $t$) take forms of the following:

$$\frac{\mathrm{d}l}{\mathrm{d}m} = \epsilon \ , \tag{1}$$

$$\frac{\mathrm{d}p}{\mathrm{d}m} = -\frac{Gm}{4\pi r^4} \ , \tag{2}$$

$$\frac{\mathrm{d}r}{\mathrm{d}m} = \frac{1}{4\pi r^2 \rho} \ , \quad \text{and} \tag{3}$$

$$\frac{\mathrm{d}t}{\mathrm{d}m} = -\frac{Gmt}{4\pi r^2 p}\nabla \ . \tag{4}$$

Thus, in my model, there are four variables $(l, p, r, t)$ and their derivatives. If the chosen stellar mass and elemental abundances are physically possible for ZAMS stars, a set of boundary conditions that satisfy the above set of differential equations should exist, and such boundary conditions should only depend on the four free parameters. The free parameters should define maximum values (i.e., the total luminosity $L$, the central pressure $P_c$, total radius $R$, and the central temperature $T_c$), as all quantities approach zero at either end (center or the surface). Integrating the differential equations while satisfying the appropriate boundary conditions by optimizing free parameters is, therefore, the goal and the challenge of this project.

### 1.1. *Energy generation*

Energy is generated by pp-chain and CNO-cycle reactions. I use an approximation made in SSE. For p-p

chain, the energy generation raate is

$$\epsilon_{pp} = 2.57 \times 10^4 \psi f_{11} g_{11} \rho X_1 T_9 {}^{-2/3} e^{-3.381/T_9^{1/3}}$$
$$g_{11} = 1 + 3.82T_9 + 1.51T_9^2 + 0.144T_9^3 - 0.0114T_0^4 \quad (5)$$

and for CNO cycle, we have

$$\epsilon_{\rm CNO} = 8.25 \times 10^{25} g_{14,1} X_{\rm CNO} X_1 \rho T_9^{-2/3} \cdot e^{(-15.23T_9^{-1/3} - T9^2/0.8^2)}$$
$$g_{14,1} = 1 - 2.0T_9 + 3.41T_9^2 - 2.43T_9^3 \ . \quad (6)$$

The screening factor is defined as

$$f = e^{E_D/kT} \quad (7)$$

and I use the weak screening:

$$\frac{E_D}{kT} = \frac{Z_1 Z_2 e^2}{r_D kT} = 5.92 \times 10^{-3} Z_1 Z_2 \left(\frac{\zeta\rho}{T_7^3}\right)^{1/2} \ . \quad (8)$$

The values of $\zeta$ and $\psi$ are taken to be the unity as an approximation, and the elemental abundance fraction is set based on the total metallicity: $X_{\rm CNO} = 0.7Z$.

### 1.2. *Equation of state*

At each location, I assume that the temperature–pressure–density relation (i.e., equation of state) follows that of an ideal gas. The ideal gas law

$$P_{\rm gas} = NkT$$

can be written as

$$\rho_{\rm gas} = \frac{P_{\rm gas}\mu m_p}{k_B T} \ , \quad (9)$$

where $m_p$ is approximately the mass of a proton. Since we have a significant amount of radiation pressure due to the high temperature, we obtain an equation of state as a function of the total pressure $P$,

$$\rho_{\rm gas} = \frac{(P - P_{\rm rad})\mu m_p}{k_B T} \ , \quad (10)$$

where $P_{\rm rad} = aT^4/3$ is the radiation pressure.

### 1.3. *Energy transport*

The generated energy is transported either by radiation or convection.

### 1.4. *Opacity*

Calculating a realistic opacity value, as a function of temperature and density, is a nontrivial task and I use an existing, state-of-the-art table for this project.

It should be noted that I also extrapolated the table beyond its original boundary, as the $\rho$–$T$ relation sometimes hits near the edge (but not too far). Extrapolating the table therefore helps avoid issues with the numerical calculation.

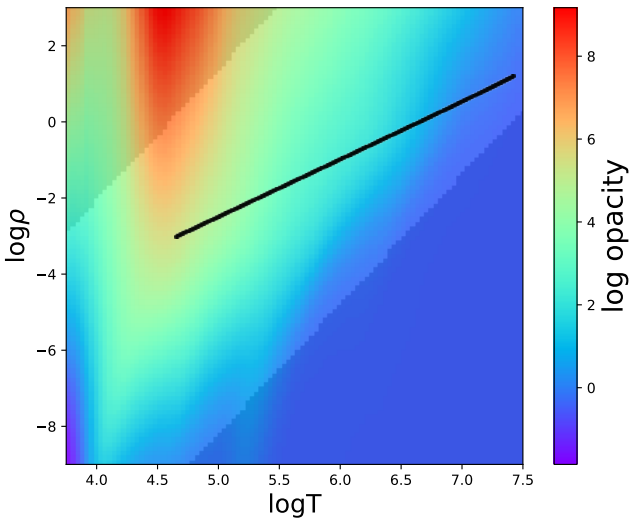


**Figure 1.** A map of the interpolated & extrapolated opacity table. Black dots represent the density and temperature values in the reported $5M_\odot$ ZAMS star.

### 1.5. *Gradient*

The actual energy transport is radiative if the radiation gradient $\nabla_{\rm rad}$ is smaller than adiabatic gradient $\nabla_{\rm ad}$. Each quantity is calculated as the following:

$$\nabla_{\rm rad} = \frac{3}{16\pi acG} \frac{P_r \kappa}{T_r^4} \frac{L_r}{M_r} \quad (11)$$

$$\nabla_{\rm ad} = \left(1 + \frac{(1-\beta)(4+\beta)}{\beta^2}\right) / \left(\frac{5}{2} + \frac{4(1-\beta)(4+\beta)}{\beta^2}\right) \quad (12)$$

When the radiation pressure is not negligible (i.e., the gas pressure fraction $\beta \equiv P_{\rm gas}/P_{\rm total}$ is unity), the adiabatic gradient deviates from the ideal gas–only value of $\sim 0.4$.

## 2. BOUNDARY CONDITIONS

### 2.1. *Center*

At the very center, by definition, we have $r = 0$ and $l = 0$. Zero values, however, cause difficulties with the numerical integration. Instead, we choose a region right outside the center at the enclosed mass of `M_i` and I calculate corresponding quantities following the constant-density core model described in SSE.

Calculating the luminosity and the enclosing radius at this coordinate is relatively straightforward, assuming constant density, as

$$R_i^3 = \frac{3M_i}{4\pi\rho_c} \ , \quad (13)$$
$$L_i = \epsilon(T_c, \rho_c) \cdot M_i \ . \quad (14)$$

The energy generation rate $\epsilon$ and density $\rho_c$ are calculated from the proposed free parameters ($P_c$,$T_c$). The radius enclosing $M_i$ is

The pressure at this coordinate is

$$P_i = P_c + \frac{3G}{8\pi}\left(\frac{4\pi}{3}\rho_c\right)^{4/3} m^{2/3} \ . \tag{15}$$

The density $\rho_c$ is calculated from the proposed free parameter $P_c$ and $T_c$, assuming that the density does not change rapidly at the core.

The temperature at this coordinate takes different forms depending on the energy transfer methods. First the gradient values $\nabla_{\rm rad}$ and $\nabla_{\rm ad}$ are calculated using the proposed free parameters ($P_c$,$T_c$). The temperature values are calculated as the following:

$$T_i = \begin{cases} \left[T_c^4 - \left(\frac{3}{4\pi}\right)^{2/3} \frac{\kappa_c \epsilon_c \rho_c^{4/3} m^{2/3}}{2ac}\right]^{1/4} & , \nabla_{\rm rad} =< \nabla_{\rm ad} \\ \exp\left[\ln T_c - \left(\frac{\pi}{6}\right)^{1/3} \frac{G\nabla_{\rm ad}\rho_c^{4/3} m^{2/3}}{P_c}\right] & , \nabla_{\rm rad} > \nabla_{\rm ad} \end{cases} . \tag{16}$$

The inner boundary condition is, therefore,

$$(l, p, r, t) = (L_i, P_i, R_i, T_i) \ . \tag{17}$$

### 2.2. *Surface*

I define the surface of a star at the photosphere. Folloging chapter 11.3 in SSE, I employ the Eddington gray atmosphere; i.e., $T = T_{\rm eff}$ and $P = P(\tau = 2/3)$. An assumption, that the fraction of mass outside photosphere is negligible, immediately provides the boundary condition for radius $R_s = R$ and $L_s = L$. This is followed by the calculation of effective temperature:

$$T_s = T_{\rm eff} = \left(\frac{L}{4\pi R^2 \sigma_{\rm SB}}\right)^{1/4} \ . \tag{18}$$

For the integration of the differential equation for pressure, a solution of the differential equation of the pressure above photosphere along the optical depth provides a good approximation:

$$\frac{{\rm d}P}{{\rm d}\tau} = \frac{GM}{R^2 \kappa(T_{\rm eff}, \tilde{\rho})} \tag{19}$$

where $\tilde{\rho} = \rho(P, T_e f f)$ is a function of $P$, which makes this into an ordinary differential equation. This ODE is solved with the initial condition $P(\tau = 0) = P_{\rm rad}$, and the end value $P_s = P(\tau = 2/3)$ is taken as the boundary condition for the surface of the star. The resulting boundary conditions are, therefore,

$$(l, p, r, t) = (L, P_s, R, T_{\rm eff}) \ . \tag{20}$$

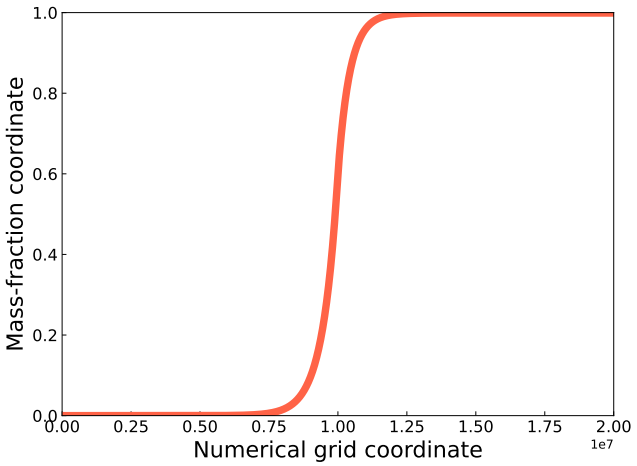


**Figure 2.** Assignment of grid points.

## 3. NUMERICAL CALCULATION

### 3.1. *Integrating differential equations*

I use `scipy.integrate.odeint` to integrate differential equations with initial values. With a sufficiently dense gridpoints (discussed in Sec. 3.3), this produces a smooth solution.

### 3.2. *Shoot to a fit point*

Two boundary conditions, at the near-center and the surface, cannot be given to the ODE solver directly. Instead, we can integrate the differential equations towards the midpoint ("fit point") from both sides with one set of initial values each. This method is called "shoot to a fit point". When the boundary conditions (derived from the free parameters each)

### 3.3. *Mass shell size*

It is evident from the sample plots in textbooks (and also I learned in the class) that the gradients tend to get steep near the center and the surface. This means that, to avoid numerical errors, it is better to have a more tightly spaced grid points in the mass space ("mass shell"). I use `np.geomspace()` to generate a logarithmic scale in the separations at an order of `grid_log_scale` for both at the center and at the surface (`grid_log_scale` $= (10^8, 10^{10})$, respectively). This produces the mass-fraction profile of Fig. 2, which has a desired feature of tightly packed edges without requiring substantial computing time for the midpoint. The number of the total grid is set to $2 \times 10^7$.

### 3.4. *initial guesses*

I use a constant-density model for initial guesses (from the SI textbook). Using the homology relation for the

constant-density model, I obtain the radius and the luminosity:

$$\frac{R_{\rm guess}}{R_\odot} = (\frac{M_*}{M_\odot})^{0.75} , \tag{21}$$

$$\frac{L_{\rm guess}}{L_\odot} = (\frac{M_*}{M_\odot})^{3.5} . \tag{22}$$

Using these values, the central pressure and temperature are calculated as

$$P_{c,\rm guess} = \frac{3GM_*^2}{8\pi R_{\rm guess}^4} , \tag{23}$$

$$T_{c,\rm guess} = \frac{GM\mu}{2R_{\rm guess}N_A k_B} . \tag{24}$$

### 3.5. *Optimization*

When the boundary conditions at both ends are satisfied and the equations are consistent with each other, the residual at the fit point is minimized. Therefore the optimization of four free parameters is, in theory, achieved by minimizing the residual. To avoid rounding errors, I normalize the free parameters to the order of unity (which are then brought back to the physical units inside the actual calculation) and define the cost function in the form of pseudo-$\chi^2$ as

$$\chi^2 = \sum_i \frac{(y_{i,\rm L} - y_{i,\rm R})^2}{\sigma_i^2} , \tag{25}$$

where $\sigma_i$ are the normalization scales (e.g., the maximum values at either inner or outer boundary). At least one of the normalization scales must be chosen at the surface boundary condition to penalize the optimizer from choosing all the free parameters at zero.

I use `scipy.optimize.minimize` to perform optimization. To further assure that the chosen values are physical, the top-hat prior (i.e., bounds for free parameters) is set at an order of magnitude below and above the initial guesses.

## 4. MESA CALCULATION

The installation of MESA failed after a few days of attempts, so I am using the ZAMS property table from the textbook to qualitatively compare the results.[1]

## 5. RESULTS

The calculated results are shown in Fig. 3. This result was generated, however, with a few alternations in the methods from initially intended and described in the previous sections. First, despite the outward integration working and the values approaching the surface boundary condition when appropriate free parameters are proposed, the inward integration never returned a smooth, physical curve. This necessitated a change of the fit coordinate from an arbitrarily chosen midpoint to the surface boundary so that the outward integration spans the entire mass fraction range. This method is explicitly coded as the `shoot_outer()` function. Conse-

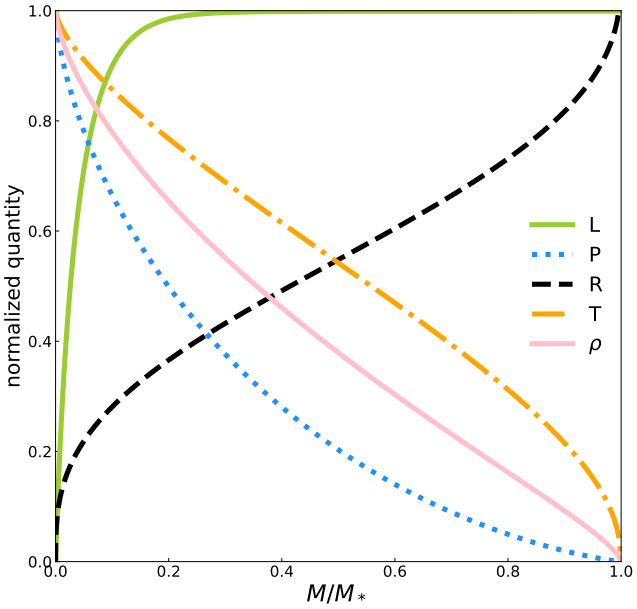


**Figure 3.** The calculated profile. The values are normalized to the maximum (either at the center or at the surface) values, which are reported in the header of the table in Appendix A.

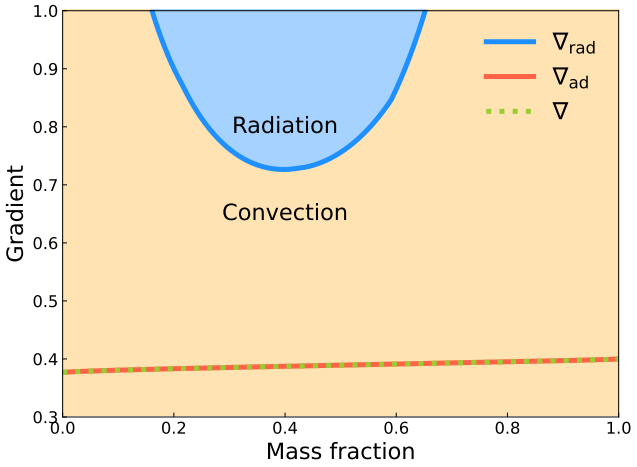


**Figure 4.** Temperature gradient and the method of energy transportation. The actual gradient $\nabla$ is below the radiative gradient and following adiabatic gradient, indicating that the star is fully convective.

[1] I spent way too much time on this project overall.

| Parameter | This work | Reference (SI) |
|---|---|---|
| $M/M_\odot$ | 5.0 | 5.0 |
| (X,Y,Z) | (0.70,0.26,0.04) | (0.74,0.24,0.02) |
| $L/L_\odot$ | 1260 | 592 |
| $R/R_\odot$ | 1.34 | 2.46 |
| $P_c/10^{16}$ (dyne/cm2) | 5.60 | 6.92 |
| $T_c/10^7$ (K) | 2.65 | 2.64 |

**Table 1.** The comparison between this work and the ZAMS properties listed in SI.

quently, the fit evaluation is not between the integrated final values but between the final (i.e., surface) value of the outward integration and the boundary condition.

Despite this change, the optimizer did not perform as expected. The optimizer failed to find the best-fit value that reduces the cost function, possibly due to the small range of the optimal regime where the gradient is smooth. As a result, I performed a "fit-by-eye" to produce the results presented in this report. The final values are confirmed to be within 5% error of the corresponding values.

The function of the optimizer and the "shoot to the fit" function are both tested using a set of simple, mock differential equations to confirm that it is not due to the coding error. Similarly, the differential equations are tested near the boundary values to confirm that it produces finite gradients in the expected directions of the slope.

The normalized profiles (Fig. 3) of calculated quantities follow the intuitive understanding of a ZAMS star: a high temperature and pressure at the center at the core, where most of the luminosity is generated; a gradual decrease in density, pressure, and temperature; and the steeper slopes in nearly all quantities at the boundaries.

The profiles of radiative, adiabatic, and actual gradient values suggest that this star is fully convective. The radiation gradient is always too large at any mass fraction point.

We compare the values to the ZAMS property tables in the SI textbook, Chapter 2, as the chosen parameters have a similar set of elemental abundances. The values are presented side-by-side in Table 1. All values are within a factor of $\sim 2$, and interior conditions have good agreements.

## 6. CONCLUSION

I performed a calculation of a five-solar mass ($5M_\odot$), zero-age main sequence (ZAMS) star with the elemental abundances of $(X, Y, Z) = (0.70, 0.26, 0.04)$ by numerically integrating four coupled differential equations and respecting the physically-motivated boundary conditions. The equations and the numerical methods worked as intended except for the inward integration from the surface, which posed difficulty with the automated optimization. Using the outward integration from near the center and adjusting parameters manually, I estimate the radius $R$ and luminosity $L$ to be $1.34R_\odot$ and $1.26 \times 10^3 L_\odot$, respectively. The interior of the star followed the intuitive understanding of the ZAMS star, and it was shown that a $5M_\odot$ star is fully convective, possibly due to the luminosity being too large to maintain stability with radiative transfer.

The main reason for many difficulties with numerical integration is most likely the failed inward integration: as the values vanish down (or plateau) near the surface, the extreme (or flat) gradient of the profile curves could make the "potential well" of the cost function very narrow and steep when the optimization is performed at the edge (i.e., "shoot to the surface" method I employed as a workaround). With the inward integration working, this would not be the case, as it allows me to revert back to the "shoot to the fit point" method, and generally the gradient is stable and the values are at the order of magnitude of the normalizing scale at the midpoint. While the exact reason of the failure for the inward integration is unclear, the first task upon the next attempt to improve this project would certainly be finding some example code whose inward integration is working.

## 7. DATA AVAILABILITY

The code and figures are all available under https://github.com/SterlingYM/stellar_structure.

# APPENDIX

## A. GENERATED TABLE

A table of calculated values are available in the GitHub repository. The format is as follows:

```
# fitted_5Msun_X70_Y26_Z04.csv
# Stellar Structure Calculation
# Yukei S. Murakami @ Johns Hopkins University, May 2023
#
# A csv file containing calculated stellar structure.
# Values with _frac are reported in the form of fraction.
```

```
# To convert to the physical unit, multiply by the scale values below.
#
###### Physical value scaling:
# mass:        m = M_frac * 5.000 * M_sun = M_frac * 5.000 * 1.988e33 [g]
# luminosity:  l = L_frac * 4.815e36 [erg/s]
# pressure:    p = P_frac * 5.597e16 [dyne/cm2]
# radius:      r = R_frac * 9.813e10 [cm]
# temperature: t = T_frac * 2.645e7  [K]
#
###### Additional quantities (calculated from the result):
# log10(rho): log density log10(rho/[g/cm3])
# log10(eps): log energy generation rate log10(eps/[erg/g])
# log10(kappa): opacity
# grad_rad: radiative gradient
# grad_ad: adiabatic gradient
# grad_actual: actual gradient d(lnT)/d(lnP)
# conv?: 1 (True) if convective, 0 (False) if radiative
#
# The structure quantities are calculated by minimizing the disagreements
# at the surface (shoot to the surface).
#
###### Fitted values:
# total luminosity:    L   = 4.819e36 [erg/s]
# central pressure:    P_c = 5.597e16 [dyne/cm2]
# photosphere radius:  R   = 9.3e10   [cm]
# central temperature: T_c = 2.645e7  [K]
#
# Additional parameters used for the calculation are available below:
#
###### Fixed values:
# abundances: X = 0.700
#             Y = 0.260
#             Z = 0.040
# molecular weight: mu = 0.615
# inner mass fraction: M_i_frac = 1e-20
# outer mass fraction: M_f_frac = 0.999
# coordinate of fitpoint(*): M_fit_frac = 0.6
#
#
# (*) since shoot-to-fit method failed for this calculation,
#     this value is only used as the coordinate of the
#     largest-spacing of the mass-shell grid.
#
M_frac,L_frac,P_frac,R_frac,T_frac,log10(rho),log10(eps),log10(kappa),grad_rad,grad_ad,grad_actual,conv?
1.000e-20,3.467e-19,1.000e+00,1.176e-07,1.000e+00,1.188e+00,4.225e+00,-3.329e-01,3.517e+00,3.767e-01,3.767e-01,1
1.106e-11,3.835e-10,1.000e+00,1.217e-04,1.000e+00,1.188e+00,4.225e+00,-3.329e-01,3.517e+00,3.767e-01,3.767e-01,1
2.215e-11,7.677e-10,1.000e+00,1.533e-04,1.000e+00,1.188e+00,4.225e+00,-3.329e-01,3.517e+00,3.767e-01,3.767e-01,1
3.325e-11,1.153e-09,1.000e+00,1.756e-04,1.000e+00,1.188e+00,4.225e+00,-3.329e-01,3.517e+00,3.767e-01,3.767e-01,1
4.437e-11,1.538e-09,1.000e+00,1.933e-04,1.000e+00,1.188e+00,4.225e+00,-3.329e-01,3.517e+00,3.767e-01,3.767e-01,1
5.552e-11,1.925e-09,1.000e+00,2.083e-04,1.000e+00,1.188e+00,4.225e+00,-3.329e-01,3.517e+00,3.767e-01,3.767e-01,1
```