MESA best practices

MESA Down Under, Sydney, 17-21 June 2024

MESA
DOWN UNDER
University of Sydney 2024

Joey Mombarg
Email: jmombarg@irap.omp.eu
Website: https://jmombarg.github.io/PersonalWebsite/index.html

Exercises: https://mesa-best-practises-sydney2024.readthedocs.io/en/latest/index.html

Starting a project

- You’re advised to use the newest MESA release.
- Check for any known bugs on the MESA docs.
- Check out the test suite for examples.
- Study the defaults files. MESA always makes a choice for physics, which is not always what you need!
  You can find these in `$MESA_DIR/star/defaults/*.defaults`
- Do convergence tests.

Converged model

- The SSE equations are solved within the tolerances used by MESA.
- The relevant physical quantities (observables) do not significantly change when increasing the resolution.

When is an iteration accepted?

- The goodness of the Newton iteration is verified by the residuals. This is the difference between the LHS and RHS of the equation.
- MESA monitors the norm (average) and max residuals.
- 3 stages of gold tolerances

```
gold_tol_residual_norm1  = 1d-11
gold_tol_max_residual1   = 1d-9
gold_iter_for_resid_tol2 = 5
gold_tol_residual_norm2  = 1d-8
gold_tol_max_residual2   = 1d-6
gold_iter_for_resid_tol3 = 10
gold_tol_residual_norm3  = 1d-6
gold_tol_max_residual3   = 1d-4
```

Verify the resolution is sufficient

- Think about required precision on the physical quantities you are interested in.
- Start for example with the default settings, and increase resolution until further increase no longer significantly changes the result.
- If that’s not the case, be aware of the numerical precision you can achieve.

Microlab 1

Microlab 1

- Front-row tables: meshing, back-row tables: time stepping
- Pick a value for `mesh_delta_coeff` (0.2-2) or `time_delta_coeff` (0.05-2), set the other one to 0.5. Coordinate with your table to have different values.
- How are the number of cells (zones) or time steps influenced?
- Which physical quantities are affected?
- What resolution would be sufficient?

Brunt-Väisälä frequency

$$N^2 = g\left(\frac{1}{\Gamma_1}\frac{\mathrm{d}\ln P}{\mathrm{d}r} - \frac{\mathrm{d}\ln\rho}{\mathrm{d}r}\right)$$

Microlab 1 setup

- Copy `$MESA_DIR/star/test_suite/1.5M_with_diffusion`
- In the `&star_job` section of `inlist_1.5M_with_diffusion`, add

```
write_profile_when_terminate = .true.
filename_for_profile_when_terminate = 'LOGS/mdcX_tdcY_nomaxdt/
profile_mdcX_tdcY_nomaxdt_Xc010.data'
```

- In the `&controls` section of `inlist_1.5M_with_diffusion`, add

```
log_directory = 'LOGS/mdcX_tdcY_nomaxdt'
set_min_D_mix = .true. ! only for time_delta_coeff
min_D_mix = 1d2        ! only for time_delta_coeff
time_delta_coeff = Y
xa_central_lower_limit_species(1) = 'h1'
xa_central_lower_limit(1) = 0.1
```

- Change

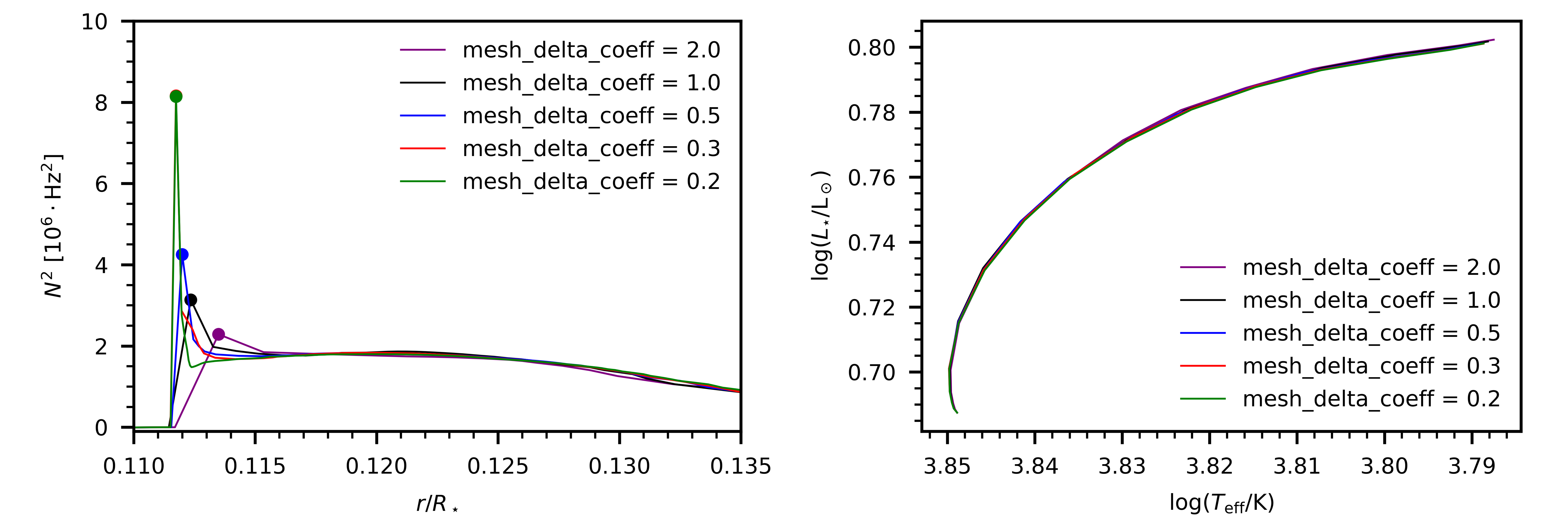
```
D_mix_ignore_diffusion = 1d10
mesh_delta_coeff = X
max_years_for_timestep = 0
max_model_number = -1
```

What does *_delta_coeff do?

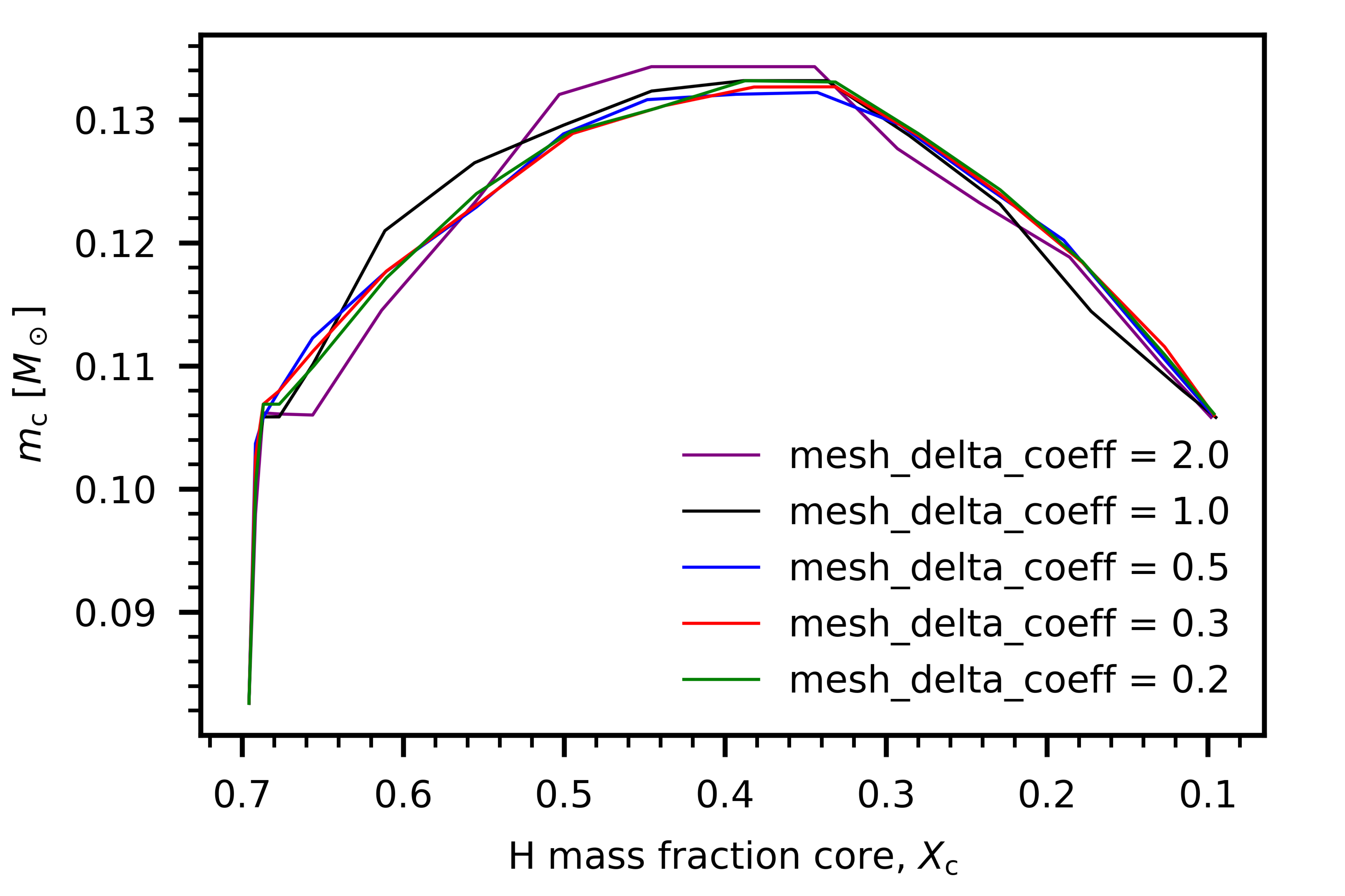
mesh_delta_coeff	time_delta_coeff	# of cells	model number
0.5	2.0	1673	48
0.5	1.0	1677	74
0.5	0.7	1654	99
0.5	0.1	1665	638
0.5	0.05	1665	1281

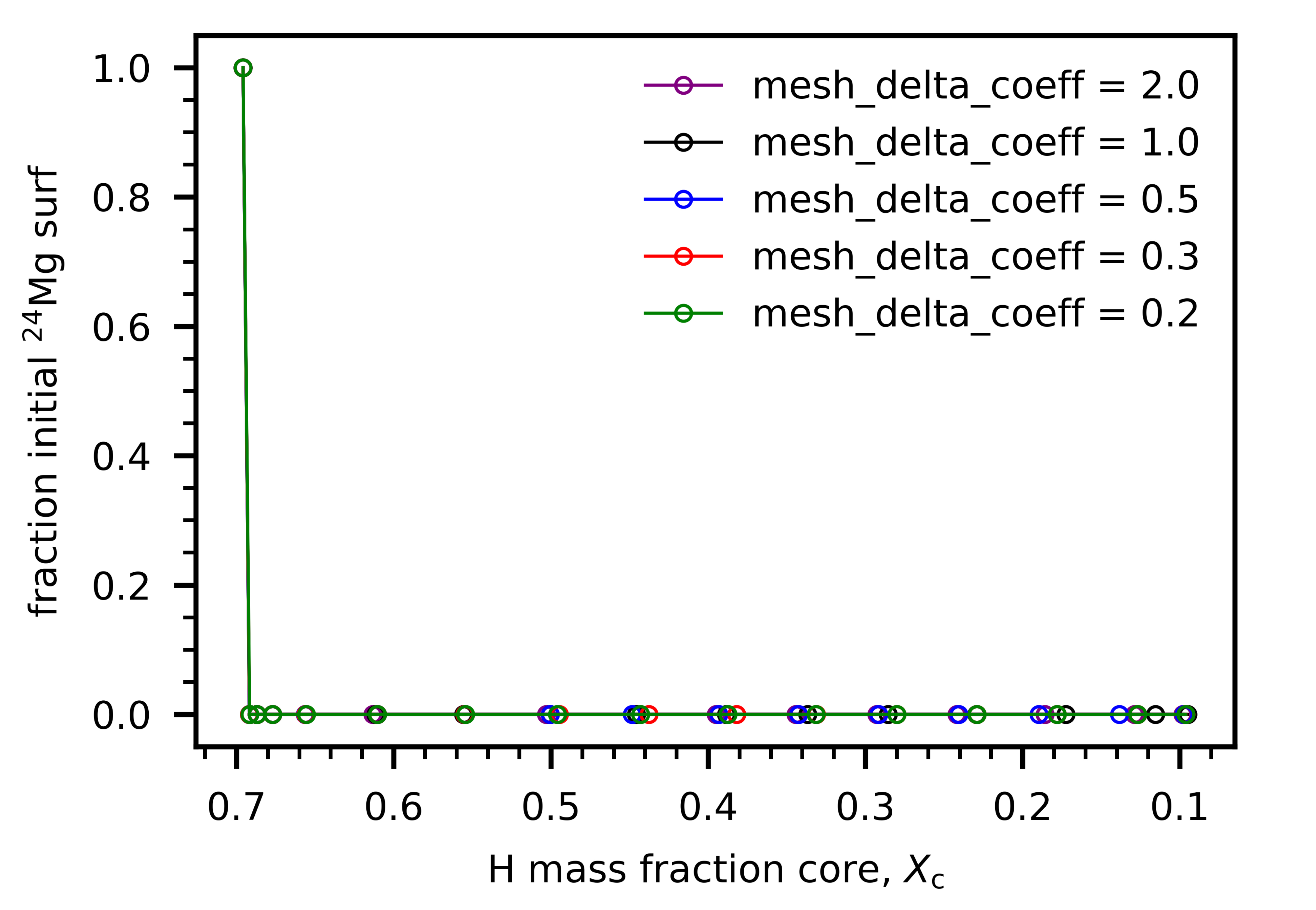
mesh_delta_coeff	time_delta_coeff	# of cells	model number
2.0	0.5	438	145
1.0	0.5	867	144
0.5	0.5	1725	148
0.3	0.5	3078	146
0.2	0.5	4458	146

Spatial resolution

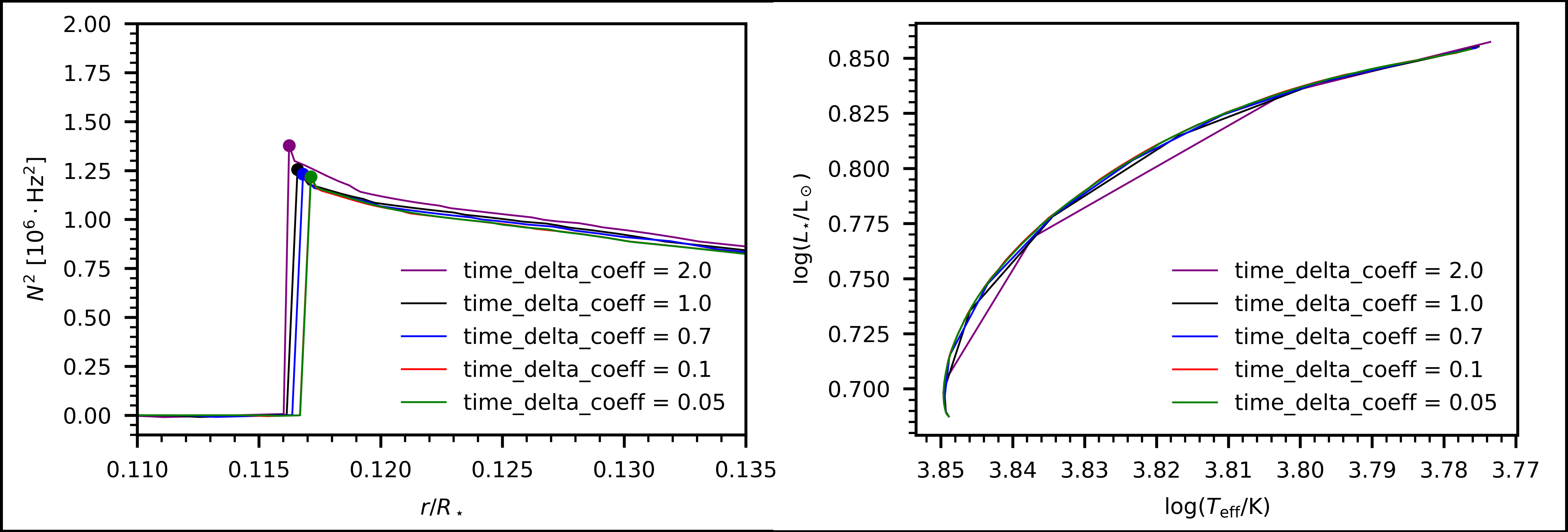


Spatial resolution

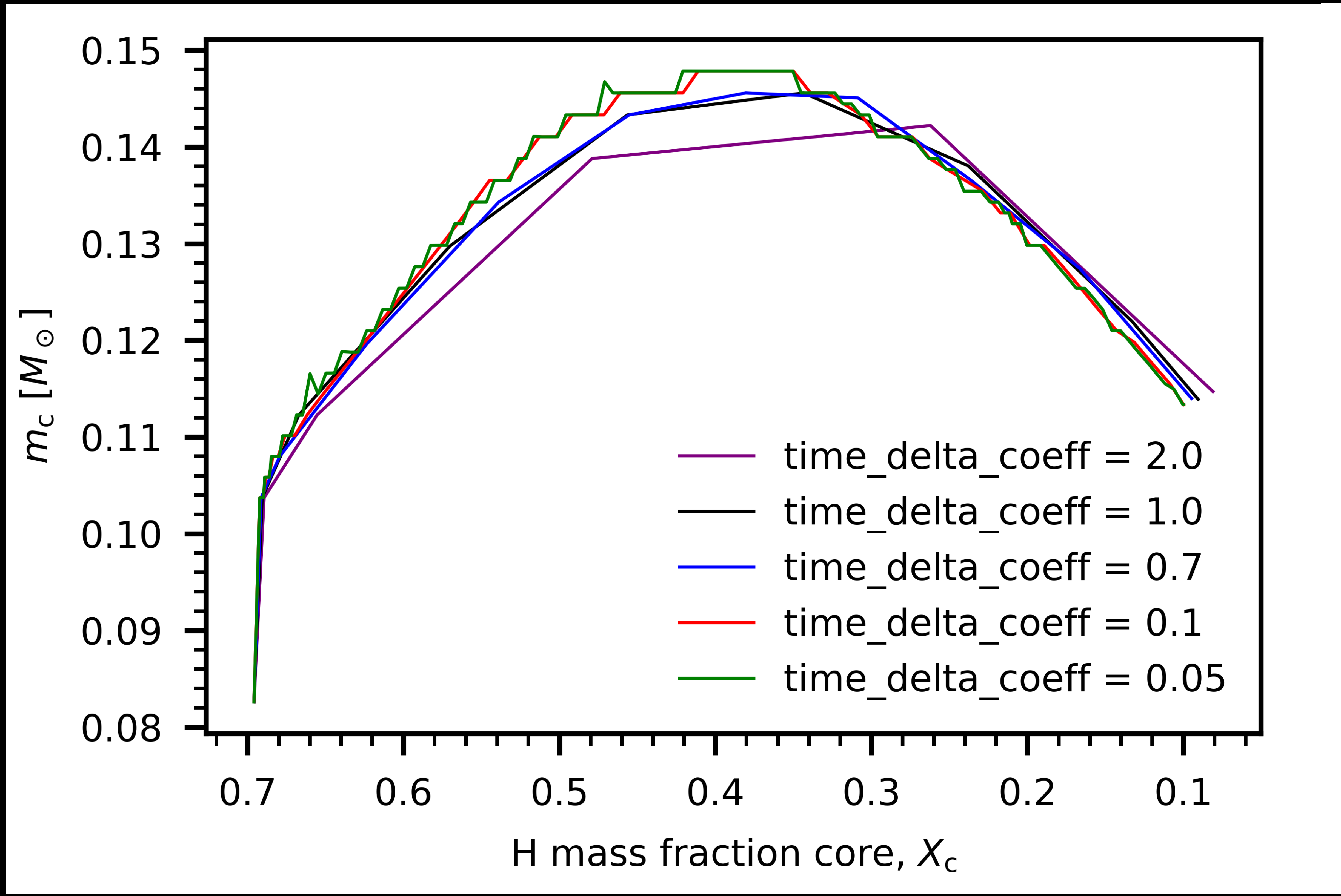


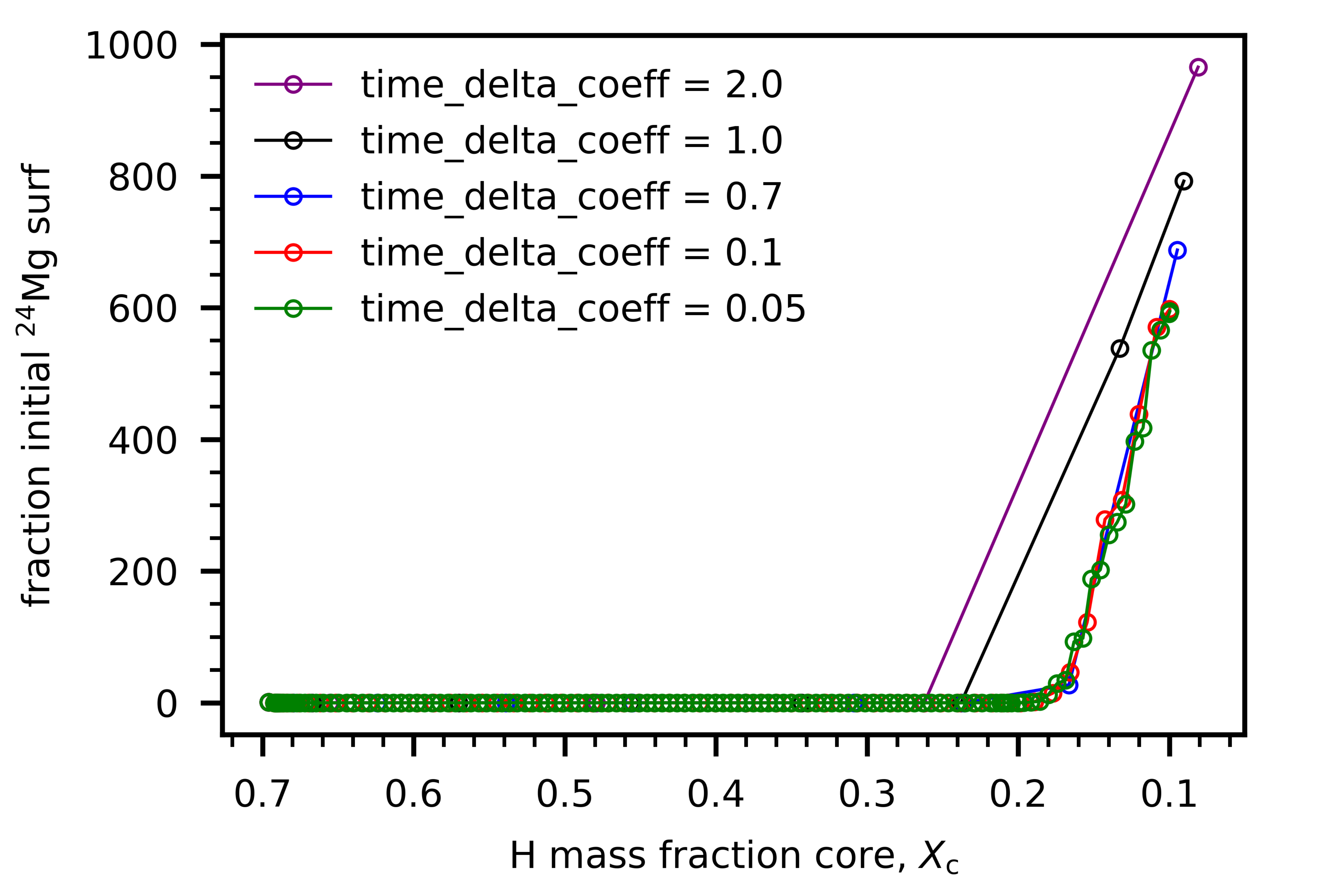


Temporal resolution



Temporal resolution





Comparing with observations

- Converting mass fractions to [X/H].
  Mention what solar composition you use.

$$[\mathrm{C/H}] = \log(X_\mathrm{C}/X_\mathrm{H}) - \log(A_\mathrm{C}/A_\mathrm{H}) - \log \epsilon_{\mathrm{C},\odot} + 12$$

- Values of $\log \epsilon_{\mathrm{X},\odot}$ can be found in `$MESA_DIR/chem/public/chem_def.f90`

```
GN93_element_zfrac(e_C)=8.55d0
GN93_element_zfrac(e_N)=7.97d0
GN93_element_zfrac(e_C)=8.87d0
```

Microlab 2

Best practices for coding in MESA

- Define double precision variables as

```
real(dp) :: your_variable ! (and not double precision :: your_variable)
```

- Numerical expressions as double

`37.0_dp` (or `37d0`)

- Exponents

`powN(x)`, or `pow(x, A)` (and not `x**N`)

- Allocate array

```
real(dp), allocatable :: arr(:)
allocate(arr(N))
deallocate(arr) ! local arrays are automatically deallocated
```

Face and cell quantities

- Examples of quantities defined at the face:
  m_k, r_k, L_k, v_k

- Examples of quantities defined at the cell:
  $\rho_k, T_k, X_{i,k}, P_k, \nabla_{\mathrm{ad},k}, \mathrm{d}m_k$

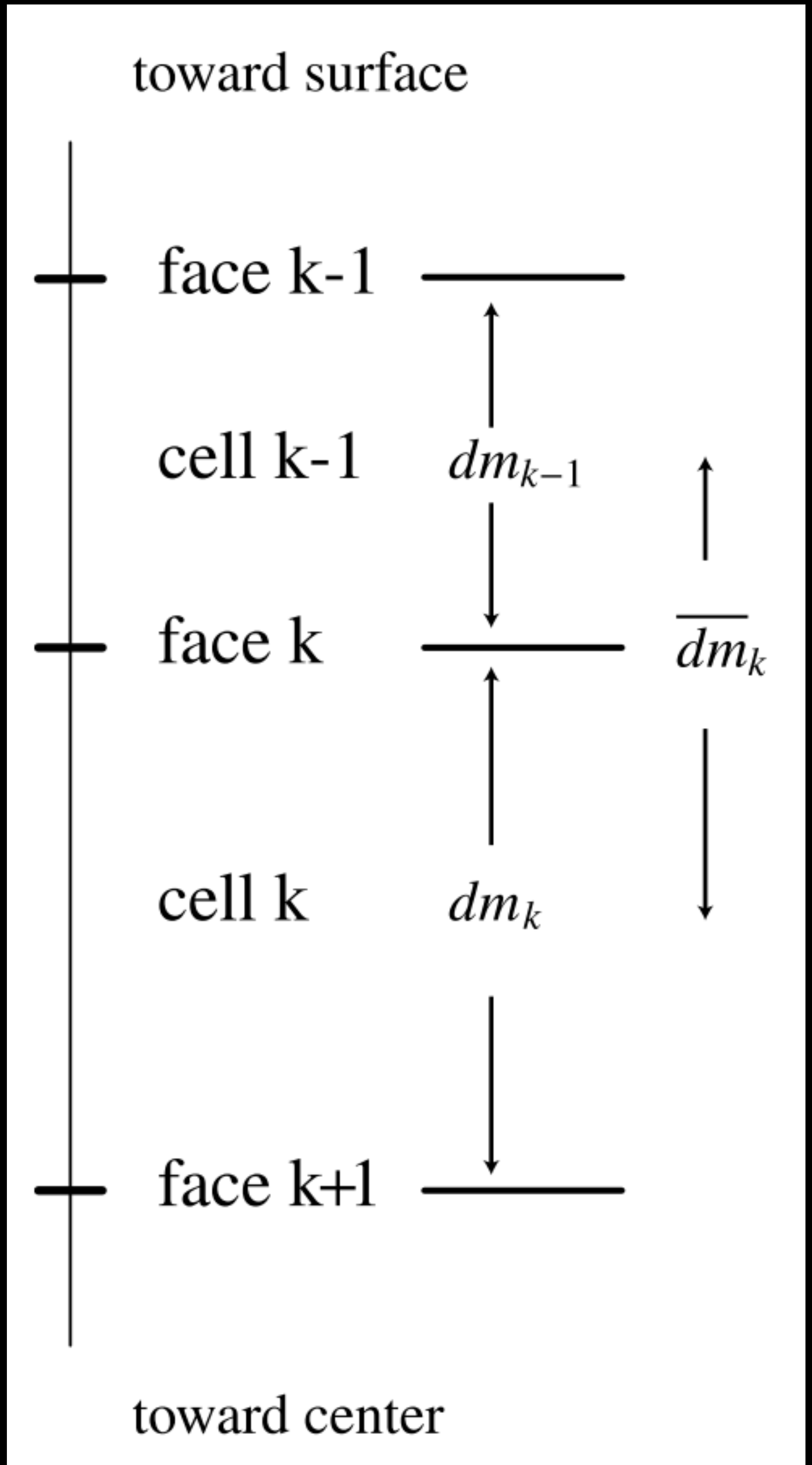


Fig. 9 in MESA Paper I, Paxton et al. (2011)

shMESA

- To enable, add `PATH=$PATH:$MESA_DIR/scripts/shmesa` to `~/.bash_profile` (or `~/.bashrc`).

`shmesa work`	copy the work directory to the current location
`shmesa change`	change a parameter in the given inlist
`shmesa defaults`	copy the history/profile defaults to the current location
`shmesa cp`	copy a MESA directory without copying LOGS, photos, etc.
`shmesa grep`	search the MESA source code for a given string
`shmesa extras`	fill in the full run_star_extras.f90 template
`shmesa zip`	prepare a MESA directory for sharing
`shmesa help`	display options

Microlab 2

- In `data_for_extra_history_columns` of the `run_star_extras.f90`, write a routine to compute the residual

$$\max\left(\frac{\left|\frac{\partial P}{\partial m} - \frac{-Gm}{4\pi r^4}\right|}{\left|\frac{\partial P}{\partial m}\right|}\right)$$

- Save the max residual of the model to a new history column “hydrostat_res”.
(Don’t forget to update `how_many_extra_history_columns`!)
Some useful functions are `maxval()`, `abs()` and `pow4()`.

- In the `&controls` section of `inlist_1.5M_with_diffusion` add

```
trace_history_value_name(3) = ‘hydrostat_res’
```

- `./clean; ./mk; ./rn`

- To what precision is hydrostatic equilibrium satisfied?

Microlab 2: result

```
allocate(residuals(s% nz))


do k = 2, s% nz
    lhs = (s% Peos(k-1) - s% Peos(k)) / ((s% dm(k-1) + s%dm(k)) / 2.0_dp)

    rhs = standard_cgrav * s% m(k) / (4.0_dp * pi * pow4(s% r(k)))

    residuals(k) = (abs(lhs - rhs)) / abs(lhs)
end do


max_residuals = MAXVAL(residuals)
names(1) = 'max_residuals'
vals(1)  = max_residuals
```

- Max residuals should be of order 10^{-7} - 10^{-9}.

When is an iteration accepted?

- The goodness of the Newton iteration is verified by the residuals. This is the difference between the LHS and RHS of the equation.
- MESA monitors the norm (average) and max residuals.
- 3 stages of gold tolerances

```
gold_tol_residual_norm1  = 1d-11
gold_tol_max_residual1   = 1d-9
gold_iter_for_resid_tol2 = 5
gold_tol_residual_norm2  = 1d-8
gold_tol_max_residual2   = 1d-6
gold_iter_for_resid_tol3 = 10
gold_tol_residual_norm3  = 1d-6
gold_tol_max_residual3   = 1d-4
```

Microlab 3

Opacities in MESA

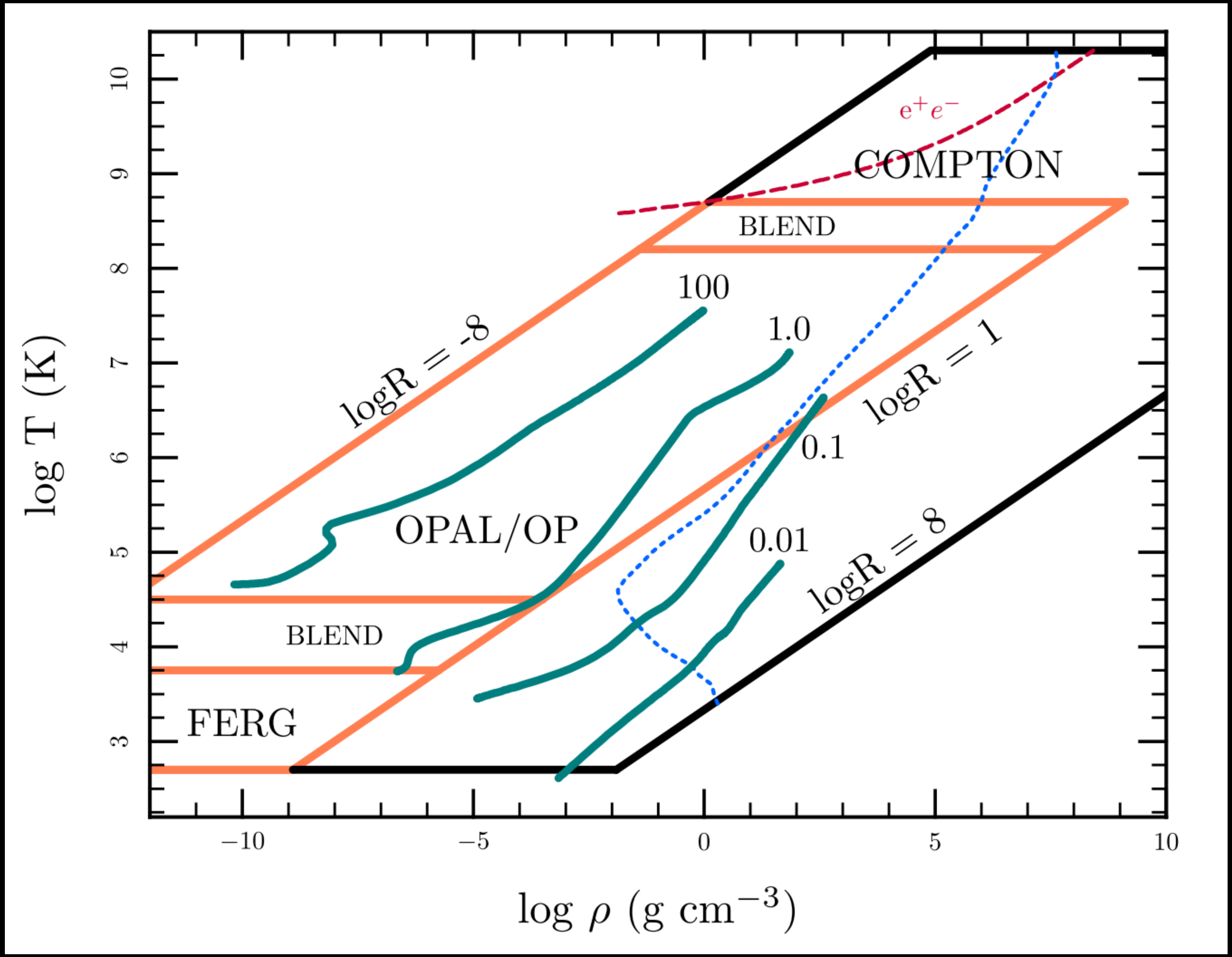


Fig. 2 in MESA Paper I, Paxton et al. (2011)

What is a mixture?

- Rosseland mean opacity

$$\kappa_\mathrm{R} = \frac{1}{\mu}\left(\int \frac{\mathrm{d}u}{\sum_k f_k \sigma_k(u)}\right)^{-1}$$

fractional abundances of chemical elements

- MESA has precomputed opacity tables assuming the relative metals fractions are fixed (to those of the Sun).

- These tables are then interpolated in X and Z.

Opacities in MESA

- Tables assume a specific mixture. It is best to be consistent with `initial_zfracs`. MESA will not complain about inconsistencies!
- By default Type 1 tables use Zbase as the reference metallicity when Z > Zbase. (Type 2 always does.) Set Zbase to the initial metallicity.

```
&kap

kap_file_prefix = ‘gs98’
kap_lowT_prefix = ‘lowT_fa05_gs98’
kap_CO_prefix   = ‘gs98_co’

Zbase = 0.02

/ ! end of kap namelist
```

Restarting

- A model can be restarted from a `.mod` file or a photo.

- Results can differ between model and photo restarts.

- `20M_pre_ms_to_core_collapse` test_suite:
  Model restart (`./rn`): final Fe core mass of 1.6816 $\mathrm{M}_{\odot}$
  Photo restart (`./rn_all`): final Fe core mass of 1.5986 $\mathrm{M}_{\odot}$

- Example of photo restart:

```
./rn_nomodfiles inlist_start_header
./re_nomodfiles . inlist_to_end_core_h_burn_header
./re_nomodfiles . inlist_to_start_he_core_flash_header
```

Microlab 3

- Copy `$MESA_DIR/star/test_suite/1M_pre_ms_to_wd`
- In `&kap` of `inlist_start`, `inlist_to_end_core_h_burn` and `inlist_to_start_he_flash` change

```
kap_file_premix = ‘’  ! Either gn93, gs98, a09, OP_gs98, or OP_a09_nans_removed_by_hand
kap_lowT_prefix = ‘’  ! Either lowT_fa05_gn93, lowT_fa05_gs98, or lowT_fa05_a09p
```

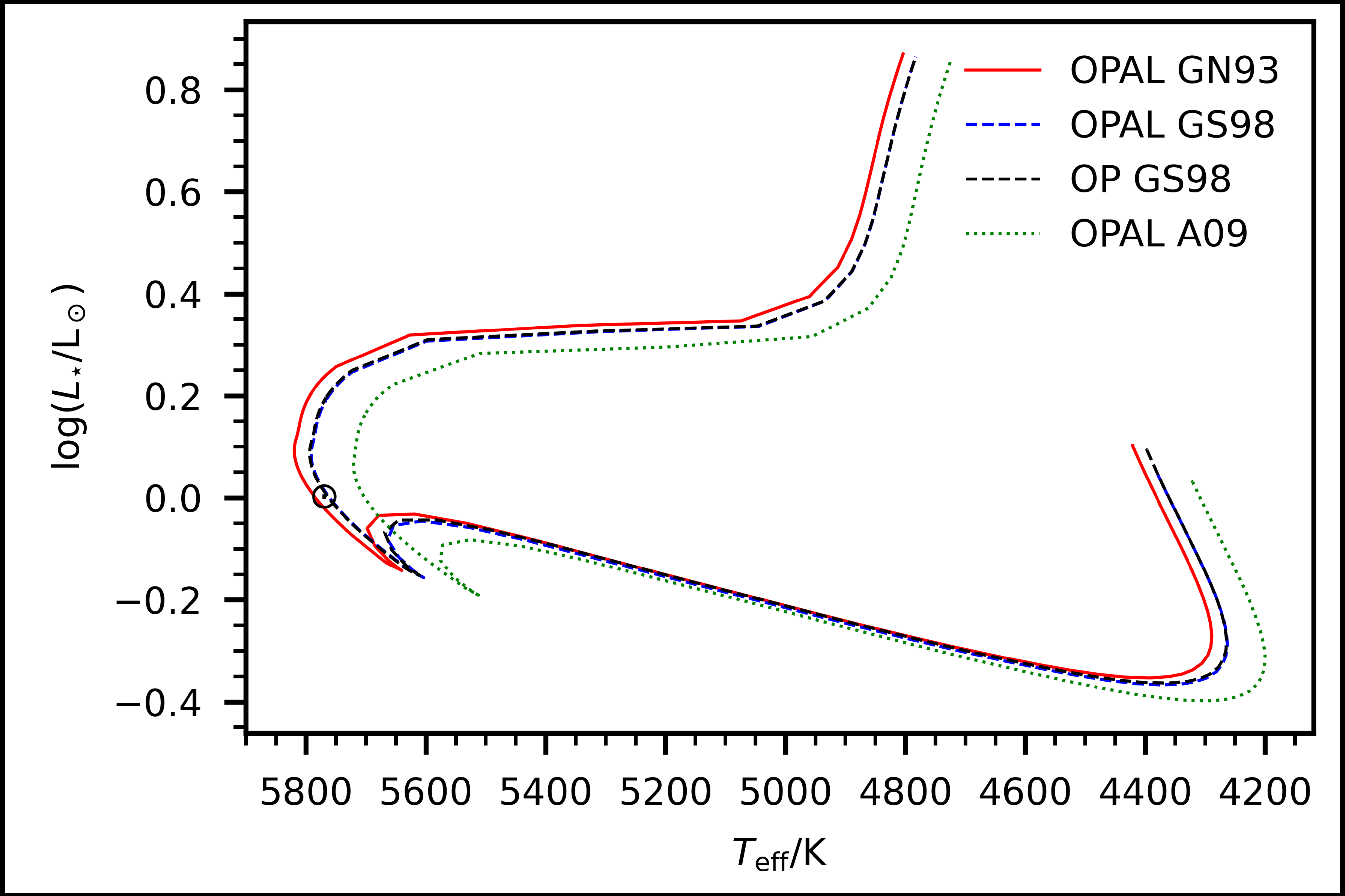
- In `&star_job` of `inlist_start` add

```
initial_zfracs = … ! 2 = GN93, 3 = GS98, 6 = A09
```

(full references can be found in `$MESA_DIR/chem/public/chem_def.f90`)

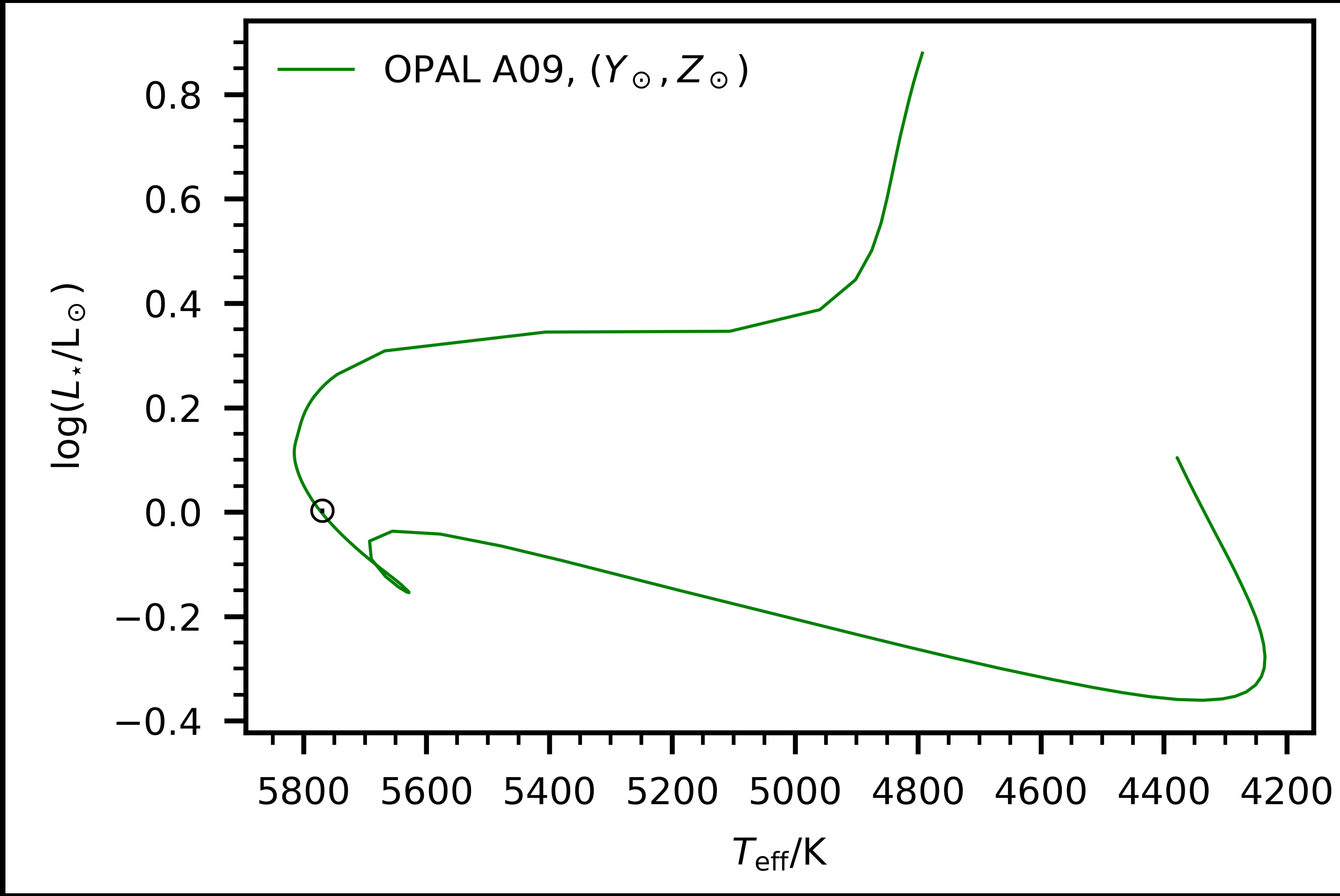
Microlab 3: result

- The choice of mixture affects the star's position in the HRD. Know how the choice affects your science case.

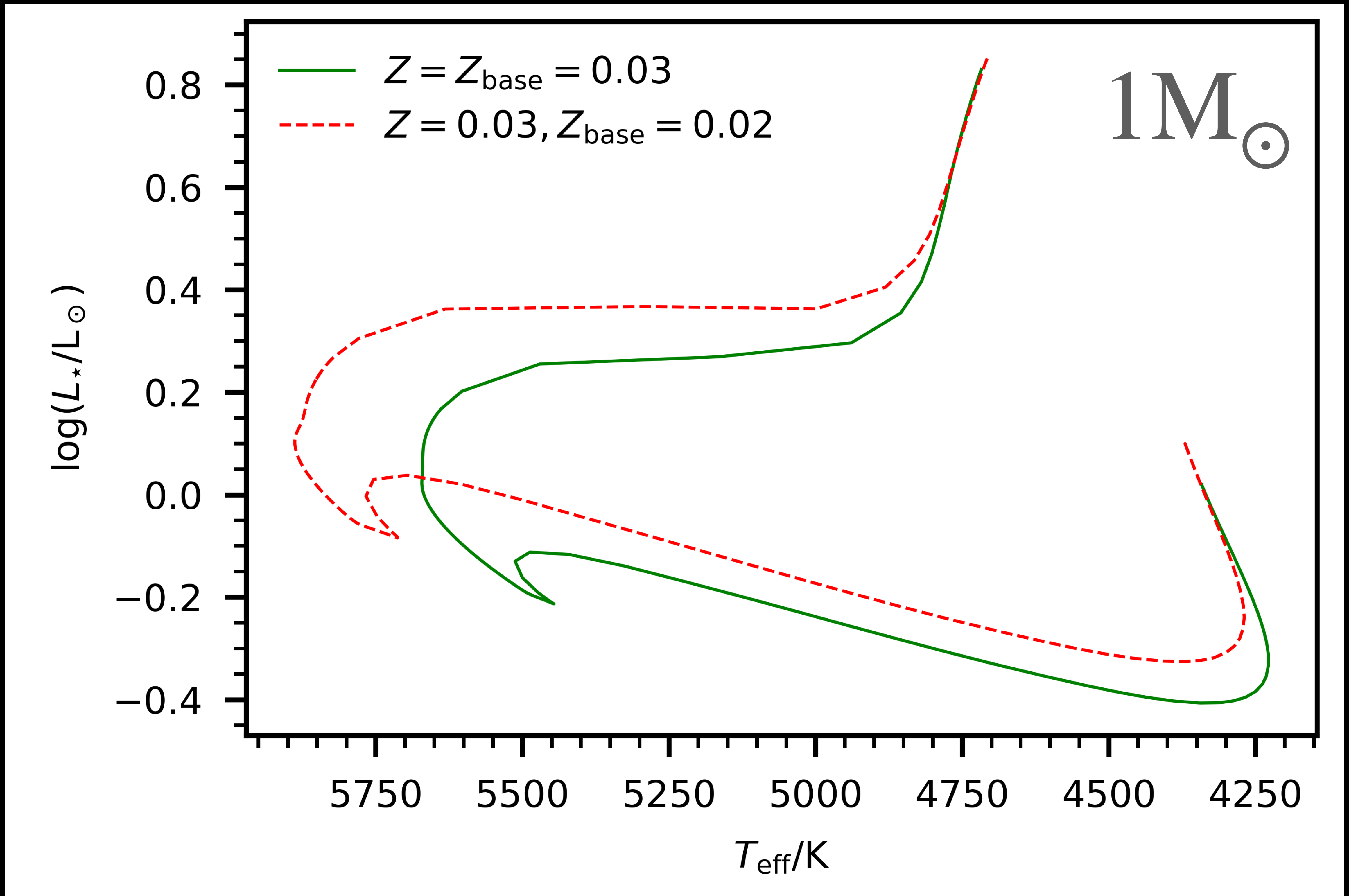


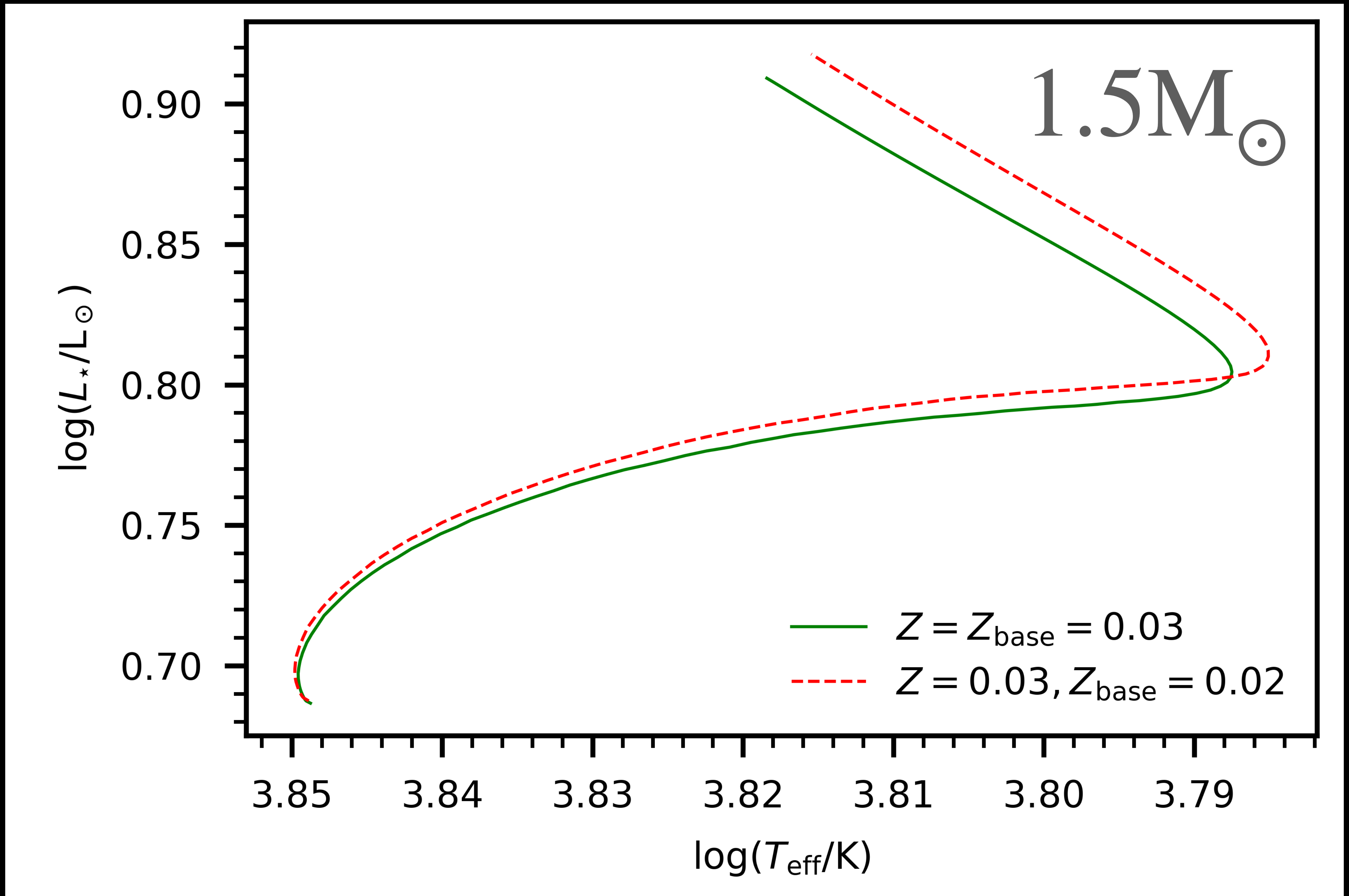
Microlab 3: result

- To intersect the Sun, also use the appropriate Y and Z for the mixture that you are using.



The effect of Zbase





HPC with MESA

- Generate a set of inlists and file with the paths

```
config=../paths_to_inlists.txt
inlist=$(awk -v ArrayTaskID=$SLURM_ARRAY_TASK_ID '$1 ArrayTaskID {print $2}' $config)
```

- Run a specific inlist with `./star inlist_name`

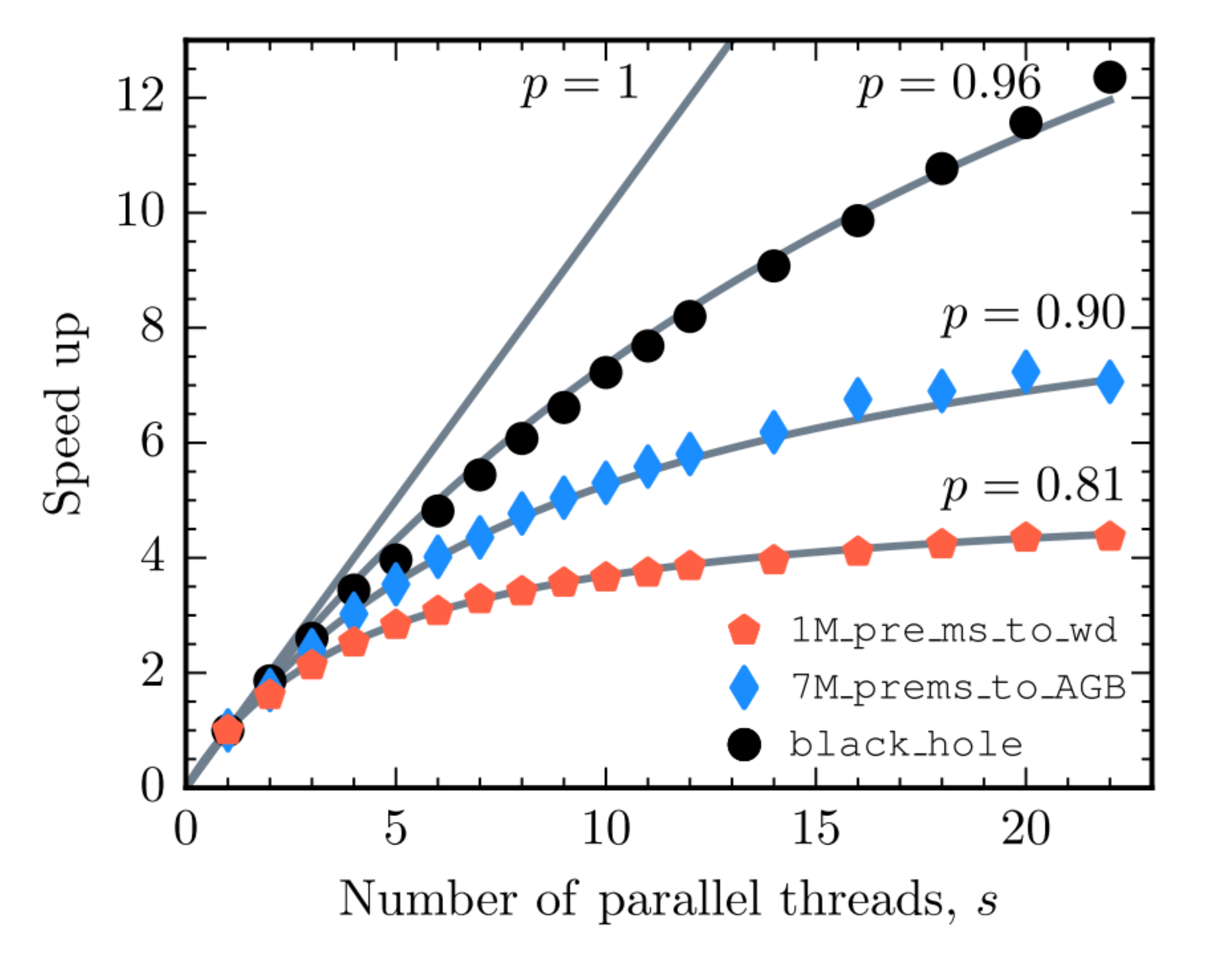
- Job array

```
sbatch job --array 0-99
```

- Make sure your work_dir is on the `$SCRATCH` disk.

HPC with MESA

- Find the optimal number of threads per run (`OMP_NUM_THREADS`).



$$\text{Speed up} = \frac{1}{(1-p) + (p/s)}$$

Fraction of code that can run in parallel

# of parallel threads

Fig. 47 in MESA Paper V, Paxton et al. (2019)

Publishing with MESA

- Always cite all MESA instrument papers at the time of your MESA version Paxton et al. (2011, 2013, 2015, 2018, 2019); Jermyn et al. (2023)
- Also consider citing the relevant microphysics

```
The MESA EOS is a blend of the OPAL \citep{Rogers2002}, SCVH
\citep{Saumon1995}, FreeEOS \citep{Irwin2004}, HELM \citep{Timmes2000},
PC \citep{Potekhin2010}, and Skye \citep{Jermyn2021} EOSes.

Radiative opacities are primarily from OPAL \citep{Iglesias1993,
Iglesias1996}, with low-temperature data from \citet{Ferguson2005}
and the high-temperature, Compton-scattering dominated regime by
\citet{Poutanen2017}.  Electron conduction opacities are from
\citet{Cassisi2007} and \citet{Blouin2020}.

Nuclear reaction rates are from JINA REACLIB \citep{Cyburt2010}, NACRE \citep{Angulo1999} and
additional tabulated weak reaction rates \citet{Fuller1985, Oda1994,
Langanke2000}.  Screening is included via the prescription of \citet{Chugunov2007}.
Thermal neutrino loss rates are from \citet{Itoh1996}.
```

Publishing with MESA

- Relevant citations for included tools

`ADIPLS`	Christensen-Dalsgaard (2008)
`GYRE`	Townsend et al. (2013, 2018); Goldstein & Townsend (2020)
`RSP`	Smolec & Moskalik (2008)
`STELLA`	Blinnikov et al. (2004, 2006), Baklanov et al. (2005)

- Cite any MESA Zenodo Community material that you use. You can also cite the MESA SDK that way.

Publishing with MESA

- Provide all material necessary to reproduce your results.
  This includes inlist, `run_star_extras/run_binary_extras`, MESA version, and MESA SDK version.

  Also consider providing computed models (profiles, history).

- A useful storage service is Zenodo. Permanent DOI, uploads to up 50Gb.
  MESA Zenodo Community

- `shMESA zip` for sharing a work directory.

“Science doesn’t have to be correct, but reproducible.”

MESA-users mailing list

- https://lists.mesastar.org/mailman/listinfo/mesa-users
- If your question concerns an error or unexpected behaviour, provide a complete work directory that reproduces the problem.
- Mention the release number, MESA SDK, and machine/OS.
- Always respond to the entire mailing list.
- Use MESA Github for reporting bugs/issues, use the mailing list for assistance.