To do the atmospheric outer boundary conds. calculations, we first need to figure out what the outermost τ, κ, T, P, ρ, R, M, & L values are.

The first block of code in the atmos.F subroutine does this.

Start w/ $d\tau = 10^{-3}$.

$M_{atm} = M_{max} - 0.9 M_{max}$ (? I think this is what the ATMASS1 & 2 are about.)

The metallicities XX & YY are given/supplied as inputs to this calculation, so we don't have to worry $\bar{c}$ determining those fr. scratch.

$d\tau_{1/2} = 1/2\, d\tau = 5\times10^{-4}$

$Itau23 = 0$

$IdelM = 0$

$R_{\tau 2/3} = R_{star}$

$z_{\tau 2/3} = M_{max}$

Note: in this code, z-variables typically refer to mass.

$T_{eff} = \left[\dfrac{L}{4\pi\sigma R_{star}^2}\right]^{1/4}$ ← L & R_{star} are also supplied as inputs, here, so we don't have to worry $\bar{c}$ calculating those fr. scratch, either.

$RK0 = 0$

$zK0 = 0$

$TK0 = \left[\frac{3}{4} T_{eff}^4 (\tau + 2/3)\right]^{1/4} = \left[T_{eff}^4 \left(\frac{3}{4}\tau + \frac{1}{2}\right)\right]^{1/2} = T_{out}$ ← in my personal notation, here

$R_{at} = R_{star}$

$z_{at} = zM(N) = M_{max}$

Next, the code claims we "define atmospheric values for JK = 1 at $\frac{1}{2} d\tau$." Do that as follows:

$P_{rad} = Crad \cdot a_{rad} \cdot TKO^4$

$P_{out} = \max\left[2 \cdot P_{rad},\ P_{rad} + 10\right]$ ← saying the outermost pressure value in the atmosphere is basically ~~st~~ set by the radiation (rather than the gas) pressure, I guess. Maybe these factors ($\times 2$, or $+10$) account in some way for the $\frac{P_{gas}}{P_{rad}}$ ratio @ this outermost point?

$\rho = \rho(T, P, XX, YY, Crad, etc.)$ ← call the eqn. of state function w/ XX, YY, P_{out} & TKO (T_{out}, basically) to find ρ

$\kappa = \kappa(N, T_{out}, \rho)$ ← call the opacity funct. to find κ as a funct. of T_{out} & ρ.

$$GD = \frac{d\tau \cdot G \cdot Z_{at}}{R_{at}^2} = \frac{d\tau \cdot G \cdot M_{star}}{R_{star}^2}$$

$$PKO = P_{out} + \frac{GD}{\kappa} = P_{out} + \frac{d\tau\, G M_{star}}{R_{star}^2\, \kappa}$$ ← $dP = P_{KO} - P_{out} = \frac{d\tau\, GM}{\kappa R^2}$

$$\left(\frac{dP}{d\tau} = \frac{GM}{R^2} \cdot \frac{1}{\kappa} \right)$$

eqn. (5.31)

Assume T doesn't change in this first outer $d\tau$ step (?). Find ρ at this new τ value as a funct. of T_{out}, PKO, XX & YY.

$\rho_{new} = \rho(T_{out}, PKO, XX, YY)$.

$\kappa_{new} = \kappa(T_{out}, \rho_{new})$

③

Still w/in the "define atmos. values for JK = 1 @ ½ dt" part of this code, we enter the following ~~for-loop~~. do-loop. (for-loop?!)

while (itr = 1, < 30, itr++):

$$GO = (PK0 - P_{out})\kappa_{new} - GD \leftarrow = dP\cdot\kappa_{new} - \frac{d\tau G M_{star}}{R_{star}^2}$$

$$PK1 = 1.001(PK0)$$

$$\rho_{K1(?)} = \rho(T_{out}, PK1, XX, YY)$$

$$\kappa_{K1(?)} = \kappa(\rho_{K1}, T_{out})$$

$$G1 = (PK1 - P_{out})\kappa_{K1} - GD \rightarrow = ((1.001-1)PK0)\kappa_1 - \frac{d\tau G M_{star}}{R_{st}^2}$$

$$\frac{dG}{dP} = \frac{G0 - G1}{PK0 - PK1} = \frac{(PK0 - P_{out})\kappa_{new} - \cancel{GD} - (PK1 - P_{out})\kappa_{K1} + \cancel{GD}}{PK0(1 - 1.001)}$$

$$= \frac{PK0\,\kappa_{new} - P_{K1}\kappa_{K1} + P_{out}(\kappa_{K1} - \kappa_{new})}{-0.001(PK0)}$$

$$dP = \frac{-G0}{dG/dP}$$

$$dP = \max(dP, -\tfrac{1}{2}PK0)$$

$$dP = \min(dP, 0.9\,PK0)$$

$$dP = \max(dP, 0.8(P_{rad} - PK0)) \leftarrow$$ is $P_{rad} - P_{K0} = P_{gas}$? why is $\frac{4}{5}P_{gas}$ an important quantity, here?

if itr > 11, $dP = \frac{1}{2}dP$. ← more forceful nudge towards convergence, I guess?

$$PK0 = PK0 + dP.$$

$$\rho_{new} = \rho(PK0, T_{out}, XX, YY)$$

$$\kappa_{new} = \kappa(\rho, T_{out})$$

if $\left|\frac{dP}{P_{K0} + P_{K1}}\right| < 10^{-5}$

then exit this loop! You've found your outer boundary conds.

After you find your outer boundary ~~conds~~ values for $\kappa, \rho, P, T, R, M,$ & L, then you go into a 4th order Runge-Kutta integration in terms of increasing values of τ. I'll ~~do~~ leave my dissection of that part of the code for later, b/c it's conceptually straightforward.

For now, I want to focus of figuring out exactly what's happening in the part of the code I just unpacked, particularly w/in the for-loop. What does it mean for those outer P, T, ρ, κ values to be "converged", physically?

Pout, Tout, Rstar, Mstar, ρout, Kout, GD

towards the center of the star

PKO, Tout, Rstar(?), M_{star}(?), ρ_{KO}, K_{KO}, GO

$= P_{out} + \frac{GD}{K_{out}}$

$\frac{dG}{dP} \rightarrow$ dP

PKl, Tout, Rstar(?), Mstar(?), ρ_{Kl}, K_{Kl}, Gl

Adjust the PKO "location" (value) using the dP value determined in this step.

$$\text{if } \left| \frac{dP}{PKO + dP + PKl} \right| < 10^{-5}, \text{ then "convergence!"}$$

$$\bar{P} = \frac{PKO + PKl}{2} \qquad \frac{1}{\bar{P}} = \frac{2}{PKO + PKl}$$

⑤

What is the purpose of this iterative PKO/PK1 process? My guess is that it's trying to bring the PKO & PK1 values closer together somehow. I also suspect that this process brings the PKO & PK1 values closer inline w/ the Pout values, although I'm less sure about that. (Need to modify the atmos.F subroutine to output values as it's doing these iterations to check how the PK1 & PKO values change wrt each other & wrt the initial P_{out} value.)

M_{star} and R_{star} (and Tout) don't change throughout this process. ρ, P, κ, & GD/G0/G1 do, however. Since GD/G0/G1 basically depend on ρ, though, that is why those values change. The amount of mass enclosed in the outermost cell depends on ρ (since neither R_{star} nor M_{star} change — this is all my guess, though), which is why the grav. accel. values at the 3 locations change.

What you're really doing in this analysis, I think, is determining the density in the outermost cell, since that sets both the opacity (κ) and thus the optical depth (τ). The density determination depends on the grav. accel. (GD/G0/G1), which in turn depends on the pressure (PK0, PK1, P_{out}(?)) x thru the $\frac{dP}{dG}$ relation.

Next step: modify the atmos.F subroutine to output info $\bar{c}$ P_{out}, PK0, PK1, densities, opacities, etc. on each pass thru the iteration loop to check/see precisely how those values evolve towards convergence or an answer or... something.