Notes on energy conservation in hydro simulations

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1 Aims

- Conserve energy (bulk kinetic+thermal+gravitational potential) to machine precision.
- This was done without particles so that gravitational PE is only due to self-gravity by Jiang et al. (2013); see also Pen (1998).
- Now I want to do this with point particles included.

2 Equations

Eq. (5) of Jiang et al. (2013) is given as

$$E_{\rm tot} = E + \frac{1}{2}\rho\phi, \tag{1}$$

where E is the sum of the bulk kinetic and thermal energy densities, ρ is mass density, and ϕ is gravitational potential. The energy equation (3) of Jiang et al. (2013) is given as

$$\frac{\partial E}{\partial t} + \boldsymbol{\nabla}\cdot[(E+P)\boldsymbol{v}] = -\rho\boldsymbol{v}\cdot\boldsymbol{\nabla}\phi, \tag{2}$$

where t is time, P is pressure, and v is bulk velocity. This can be rewritten as (Eq. (9) of Jiang et al. 2013)

$$\frac{\partial}{\partial t}\left(E + \frac{1}{2}\rho\phi\right) + \boldsymbol{\nabla}\cdot[(E+P)\boldsymbol{v} + \boldsymbol{F}_{\rm g}] = 0. \tag{3}$$

Jiang et al. (2013) derives Eq. (13) for $\boldsymbol{\nabla}\cdot\boldsymbol{F}_{\rm g}$, namely

$$\boldsymbol{\nabla}\cdot\boldsymbol{F}_{\rm g} = \boldsymbol{\nabla}\cdot\left[\rho\boldsymbol{v}\phi + \frac{1}{8\pi G}\left(\phi\boldsymbol{\nabla}\dot{\phi} - \dot{\phi}\boldsymbol{\nabla}\phi\right)\right].$$

In Jiang et al. (2013), there are no particles, so ϕ is the potential due to the gas and all potential energy is due to self-gravity of gas. Our simulation has particles and gas. Below I will demonstrate that equation (2) is still valid in this general case that includes gas and particles, with ϕ now equal to the sum of the potential due to gas and that due to particles. We will do this by repeating the derivation of Jiang et al. (2013) but keeping in mind that particles are also present.

Poisson's equation is given by

$$\nabla^2\phi = 4\pi G\rho, \tag{4}$$

and differentiating this equation with respect to time I obtain Eq. (12) of Jiang et al. 2013,

$$\nabla^2\dot{\phi} = 4\pi G\dot{\rho}. \tag{5}$$

3 The particles

For a point particle $\phi = -GM_i/|\boldsymbol{r} - \boldsymbol{r}_i|$, $\rho(\boldsymbol{r}) = M_i\delta^3(\boldsymbol{r} - \boldsymbol{r}_i)$, and $\nabla^2\phi = 4\pi GM_i\delta^3(\boldsymbol{r} - \boldsymbol{r}_i)$. But particles in the simulation are *not* true point particles because they have spline potentials. Let $u = |\boldsymbol{r} - \boldsymbol{r}_i|/h$, with h the softening radius. Then the spline potential is given by (e.g. Springel, 2010; Ohlmann et al., 2017),

$$\phi_i = -\frac{GM_i}{h}\begin{cases} -\dfrac{16}{3}u^2 + \dfrac{48}{5}u^4 - \dfrac{32}{5}u^5 + \dfrac{14}{5}, & \text{if } 0 \le u < 0.5; \\ -\dfrac{1}{15u} - \dfrac{32}{3}u^2 + 16u^3 - \dfrac{48}{5}u^4 + \dfrac{32}{15}u^5 + \dfrac{48}{15}, & \text{if } 0.5 \le u < 1; \\ \dfrac{1}{u}, & \text{if } u \ge 1. \end{cases} \tag{6}$$

Now

$$\nabla^2\dot{\phi}_i = \frac{\partial}{\partial t}\nabla^2\phi_i = \frac{\partial}{\partial t}\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\phi_i = -\frac{\partial}{\partial t}\boldsymbol{\nabla}\cdot\boldsymbol{g}_i,$$

For $\boldsymbol{g}_i = -\boldsymbol{\nabla}\phi_i = -(\partial\phi_i/\partial u)(\partial u/\partial r)\boldsymbol{\nabla}r = -(1/h)(\partial\phi_i/\partial u)\hat{\boldsymbol{r}}$ one obtains

$$\boldsymbol{g}_i = -\frac{GM_i}{h^2}\hat{\boldsymbol{r}}\begin{cases} \dfrac{32}{3}u - \dfrac{192}{5}u^3 + 32u^4, & \text{if } 0 \le u < 0.5; \\ -\dfrac{1}{15u^2} + \dfrac{64}{3}u - 48u^2 + \dfrac{192}{5}u^3 - \dfrac{32}{3}u^4, & \text{if } 0.5 \le u < 1; \\ \dfrac{1}{u^2}, & \text{if } u \ge 1. \end{cases} \tag{7}$$

Using the divergence formula in spherical coordinates $\boldsymbol{\nabla}\cdot\boldsymbol{g}_i = (1/r^2)[\partial(r^2 g_r)/\partial r]$, I compute

$$\nabla^2\phi_i = \frac{32GM_i}{h^3}\begin{cases} 1 - 6u^2 + 6u^3, & \text{if } 0 \le u < 0.5; \\ 2 - 6u + 6u^2 - 2u^3, & \text{if } 0.5 \le u < 1; \\ 0, & \text{if } u \ge 1. \end{cases} \tag{8}$$

From Poisson's equation, this implies that the particle's mass is effectively spread out over the interior of the softening sphere,

$$\rho_i = \frac{\nabla^2\phi_i}{4\pi G} = \frac{8M_i}{\pi h^3}\begin{cases} 1 - 6u^2 + 6u^3, & \text{if } 0 \le u < 0.5; \\ 2 - 6u + 6u^2 - 2u^3, & \text{if } 0.5 \le u < 1; \\ 0, & \text{if } u \ge 1. \end{cases} \tag{9}$$

Integrating this function over the volume inside the softening sphere, we recover the particle mass M_i, as expected, i.e. $4\pi\int_0^h \rho_i(r)r^2dr = 4\pi h^3\int_0^1 \rho_i(u)u^2du = M_i$.

Finally, we can compute the gravitational potential energy density of the particle as

$$\begin{aligned} \mathcal{E}_i &= \frac{1}{2}\rho_i\phi_i \\ &= -\frac{4GM_i^2}{\pi h^4}\begin{cases} -\dfrac{192}{5}u^8 + 96u^7 - \dfrac{288}{5}u^6 - \dfrac{192}{5}u^5 + \dfrac{208}{5}u^4 + \dfrac{84}{5}u^3 - \dfrac{332}{15}u^2 + \dfrac{14}{5}, & \text{if } 0 \le u < 0.5; \\ -\dfrac{64}{15}u^8 + 32u^7 - \dfrac{512}{5}u^6 + \dfrac{896}{5}u^5 - \dfrac{896}{5}u^4 + \dfrac{448}{5}u^3 - 2u^2 - \dfrac{98}{5}u + \dfrac{34}{5} - \dfrac{2}{15u}, & \text{if } 0.5 \le u < 1; \\ 0, & \text{if } u \ge 1. \end{cases} \end{aligned} \tag{10}$$

Integrating this profile over the interior of the softening sphere gives the potential energy of the particle. Making use of the results $\int_0^{0.5}\mathcal{E}_i u^2du = 0.0449324$ and $\int_{0.5}^1\mathcal{E}_i u^2du = 0.0182134$, we obtain

$$E_i = 4\pi\int_0^h \mathcal{E}_i r^2dr = 4\pi h^3\int_0^1 \mathcal{E}_i u^2du = -\frac{16(0.0631458)GM_i^2}{h} = -\frac{1.0103328GM_i^2}{h}. \tag{11}$$

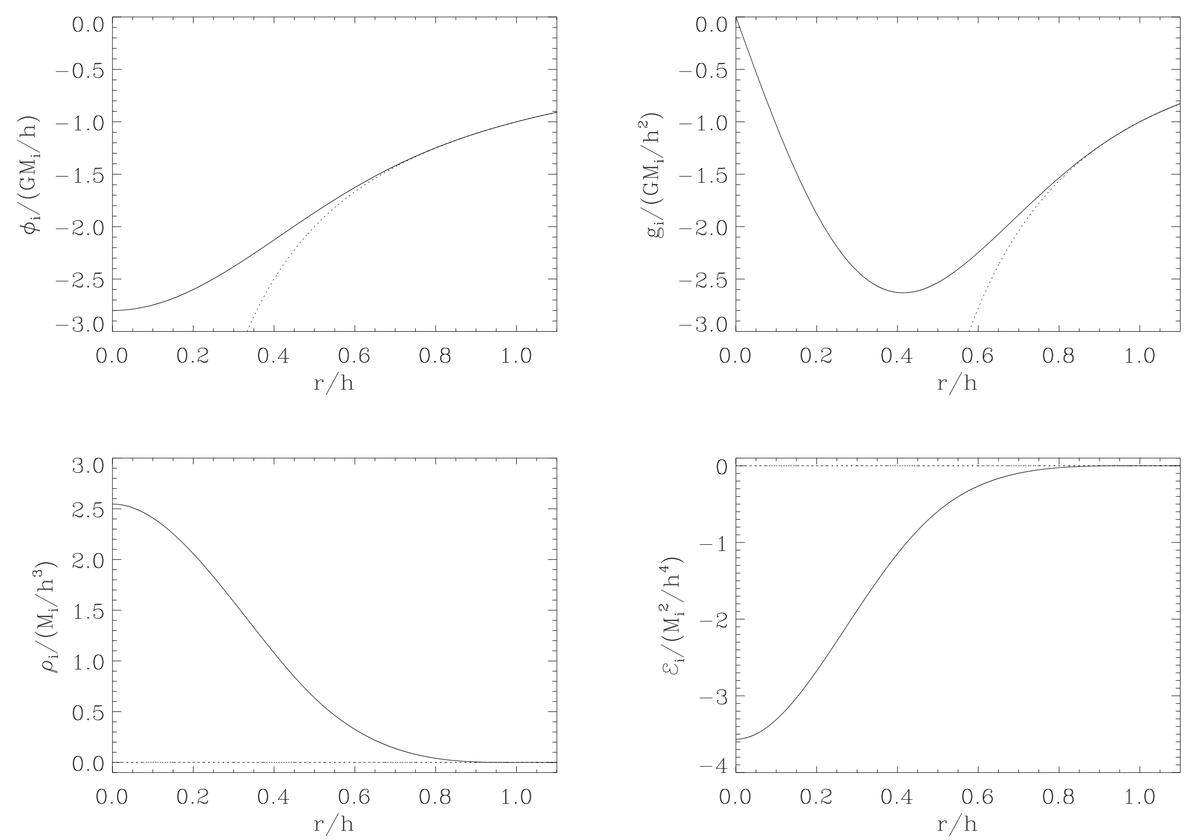

Figure 1: Solid curves show the gravitational potential, radial component of acceleration due to gravity, effective density of particle i, and effective potential energy density of particle i, a distance r from the location of the particle. Here h is the spline softening length, M_i is the particle mass, and G is Newton's constant. Dotted curves show the solution for a point particle, for comparison.

(By contrast, the potential energy of a point particle is $-\infty$.) These functions are illustrated in Fig. 1.

So in general $\rho = \rho_{\rm gas} + \rho_i$ and $\nabla^2\phi = \nabla^2\phi_{\rm gas} + \nabla^2\phi_i = \nabla^2(\phi_{\rm gas} + \phi_i)$. But outside the softening spheres, $\rho = \rho_{\rm gas}$ and $\nabla^2\phi = \nabla^2\phi_{\rm gas}$.

4 Calculation

Using Eq. (2), Eq. (3) can be written as

$$\frac{\partial}{\partial t}\left(\frac{1}{2}\rho\phi\right) + \boldsymbol{\nabla}\cdot\boldsymbol{F}_{\rm g} = \rho\boldsymbol{v}\cdot(\boldsymbol{\nabla}\phi). \tag{12}$$

The continuity equation is

$$\dot{\rho} = -\boldsymbol{\nabla}\cdot(\rho\boldsymbol{v}). \tag{13}$$

Solving for $\boldsymbol{\nabla}\cdot\boldsymbol{F}_{\rm g}$ in Eq. (12) and using Eq. (13), I obtain Eq. (11) of Jiang et al. 2013,

$$\boldsymbol{\nabla}\cdot\boldsymbol{F}_{\rm g} = \frac{1}{2}\boldsymbol{\nabla}\cdot(\rho\boldsymbol{v})\phi + \rho\boldsymbol{v}\cdot\boldsymbol{\nabla}\phi - \frac{1}{2}\rho\dot{\phi}. \tag{14}$$

Now, let's break up the first term in Eq. (14) to write

$$\boldsymbol{\nabla}\cdot\boldsymbol{F}_{\rm g} = \boldsymbol{\nabla}\cdot(\rho\boldsymbol{v})\phi - \frac{1}{2}\boldsymbol{\nabla}\cdot(\rho\boldsymbol{v})\phi + \rho\boldsymbol{v}\cdot\boldsymbol{\nabla}\phi - \frac{1}{2}\rho\dot{\phi}. \tag{15}$$

Now, using Eqs. 4 and (5) and the continuity equation (13), Eq. (15) can be written as

$$\boldsymbol{\nabla}\cdot\boldsymbol{F}_{\rm g} = \boldsymbol{\nabla}\cdot(\rho\boldsymbol{v})\phi + \rho\boldsymbol{v}\cdot\boldsymbol{\nabla}\phi + \frac{1}{8\pi G}(\phi\nabla^2\dot{\phi} - \dot{\phi}\nabla^2\phi). \tag{16}$$

Now

$$\boldsymbol{\nabla}\cdot(\phi\boldsymbol{\nabla}\dot{\phi} - \dot{\phi}\boldsymbol{\nabla}\phi) = \boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\dot{\phi} + \phi\nabla^2\dot{\phi} - \boldsymbol{\nabla}\dot{\phi}\cdot\boldsymbol{\nabla}\phi - \dot{\phi}\nabla^2\phi = \phi\nabla^2\dot{\phi} - \dot{\phi}\nabla^2\phi$$

and

$$\boldsymbol{\nabla}\cdot(\rho\boldsymbol{v}\phi) = \boldsymbol{\nabla}\cdot(\rho\boldsymbol{v})\phi + \rho\boldsymbol{v}\cdot\boldsymbol{\nabla}\phi.$$

Using these relations in Eq. (16) I obtain Eq. (13) of Jiang et al. (2013)

$$\boldsymbol{\nabla}\cdot\boldsymbol{F}_{\rm g} = \boldsymbol{\nabla}\cdot\left[\rho\boldsymbol{v}\phi + \frac{1}{8\pi G}(\phi\boldsymbol{\nabla}\dot{\phi} - \dot{\phi}\boldsymbol{\nabla}\phi)\right]. \tag{17}$$

One choice of $\boldsymbol{F}_{\rm g}$ is just the expression inside the square brackets.

We see then that the Jiang et al. (2013) derivation goes through with $\phi = \phi_{\rm gas} + \phi_i$, but only if ρ is generalized as $\rho = \rho_{\rm gas} + \rho_i$, with ρ_i given by Eq. (9).

References

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Ohlmann, S. T., Röpke, F. K., Pakmor, R., & Springel, V. 2017, A&A, 599, A5

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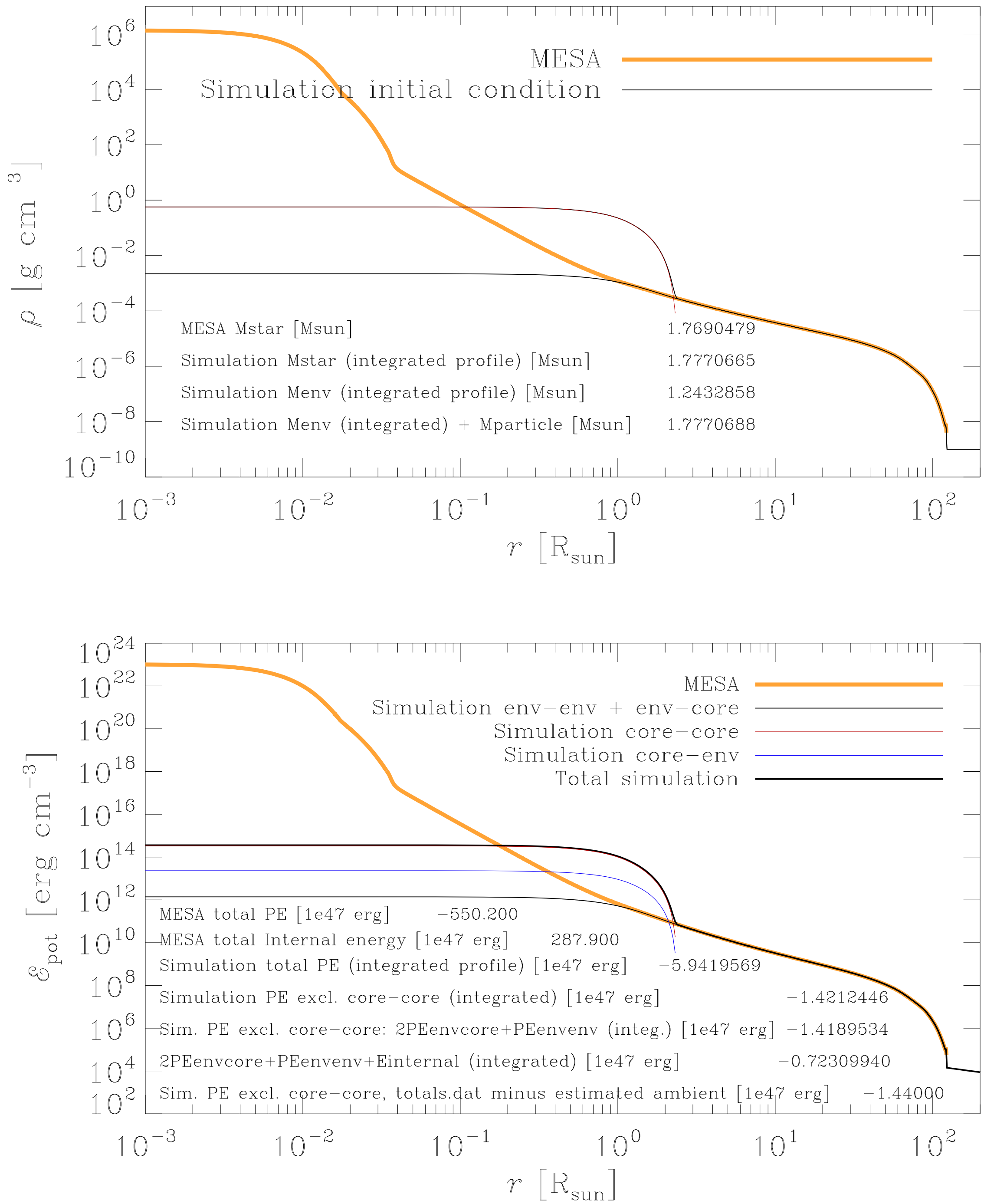

Figure 2: Density and potential energy profiles for AGB star at $t = 0$. Core profiles obtained using equations (9) and (10).

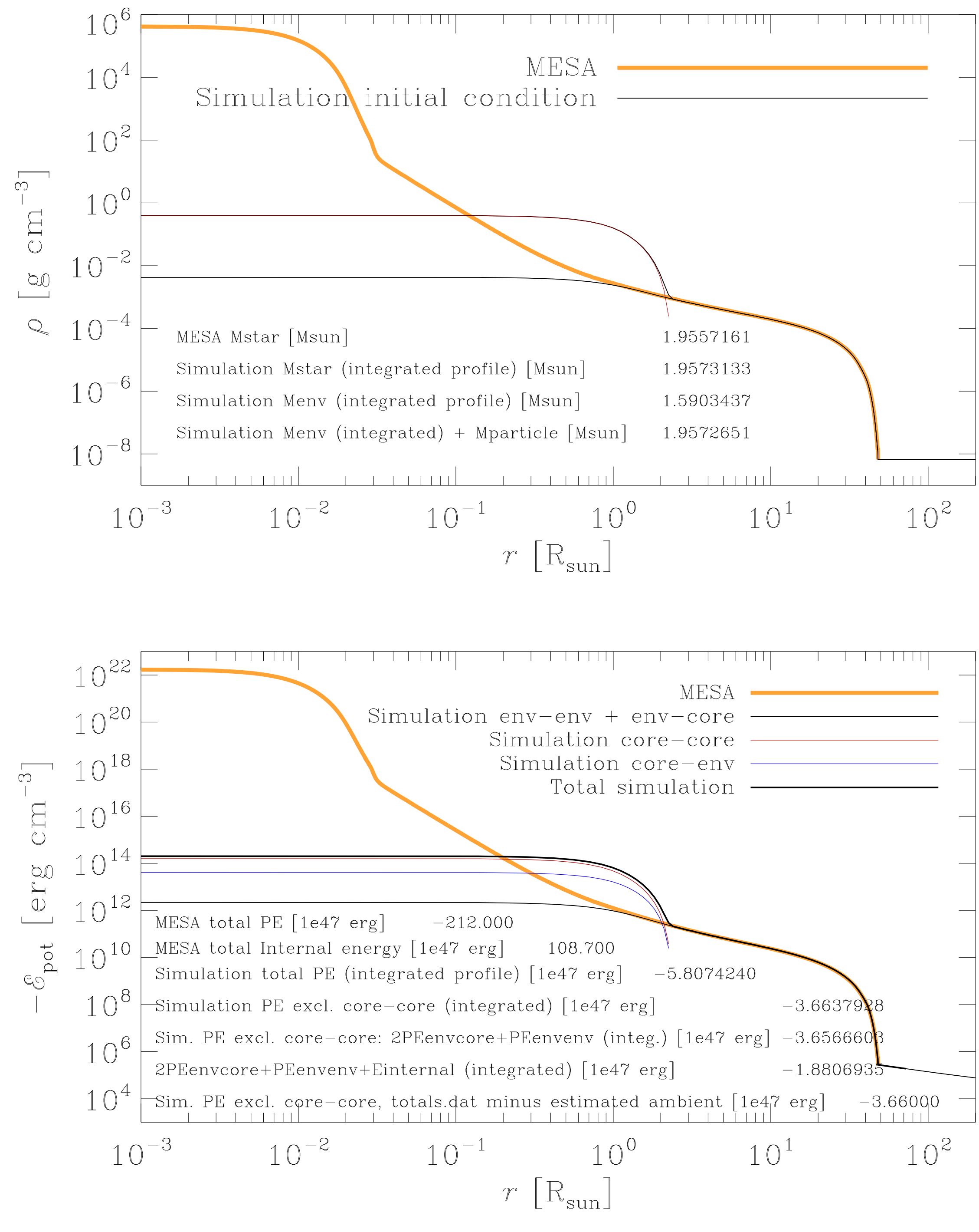

Figure 3: Density and potential energy profiles for RGB star at $t = 0$. Core profiles obtained using equations (9) and (10).