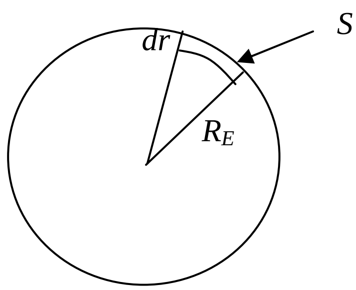
Pressure: macroscopic to microscopic

We looked at elastic properties of solids during our last lecture. We have been able to link bulk modulus to interatomic potential within the approximation of small compression at low temperature. In this tutorial we shall look at an interesting example of microscopic and microscopic pressure.

The question we ask is how pressure in the centre of the Earth would compare to interatomic one. First, we shall look at the pressure in the centre of the Earth. It is cleat that pressure will be caused by gravity. If we consider a simple approximation of Earth being a hard sphere of uniform density pressure can then be calculated by considering a small segment of the surface *S* of thickness *dr*:



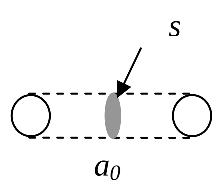
Pressure exerted by this segment is then:

$$dP = \frac{dF}{S}, F = mg = mrS\rho \Rightarrow dP = \frac{gmS\rho dr}{S} = g\rho dr$$

$$\text{while } mg(r) = G\frac{mM}{r^2} \Rightarrow g(r) = \frac{GM}{r^2} = G\rho\frac{4}{3}\pi\frac{r^3}{r^2} = G\rho\frac{4}{3}\pi r$$

$$\text{and hence } dP = \rho G\rho\frac{4}{3}\pi r dr \Rightarrow P = \frac{4}{3}\pi\rho^2\int_0^R r dr = \frac{2}{3}G\pi\rho^2 R^2$$

Now, let's turn our attention to the "interatomic" pressure. We shall define it as a pressure that corresponds to the force acting between two isolated atoms that interact via LJ potential at low T.



Pressure can then be calculated as:

$$p = \frac{f}{s} = \frac{4f}{\pi\sigma^2}, \text{ where } \sigma \text{ is atomic diameter and}$$

$$f = f_{attraction} + f_{repulsion}$$

and we can find f for LJ from

$$\left.\frac{dV}{dr}\right|_{a_0} = 48\varepsilon\frac{\sigma^{12}}{a_0^{13}} - 24\varepsilon\frac{\sigma^6}{a_0^7} = 0 \Rightarrow f = 48\varepsilon\frac{\sigma^6}{a_0^7}$$

And we can find pressure.