Research Software Engineer Apprentice – Scientific Computing Department

Assessment Task 1

Background Information:

Finding the value of total energy of a system is a typical example of tasks in scientific computing. In this problem, we wish to determine that value of a small system of charged particles. The task can be completed both by hand or by using simple code in a programming language of your choice.

The system contains 8 particles with the following positions and charges:

```
# (index) x y z (position) q (charge)
        1 +0.25 +0.25 +0.25  1
        2 -0.25 +0.25 +0.25 -1
        3 +0.25 -0.25 +0.25 -1
        4 +0.25 +0.25 -0.25 -1
        5 -0.25 -0.25 +0.25  1
        6 +0.25 -0.25 -0.25  1
        7 -0.25 +0.25 -0.25  1
        8 -0.25 -0.25 -0.25 -1
```

If we had 4 particles 1, 2, 3, 4 then there are the 6 pair interactions 1-2, 1-3, 1-4, 2-3, 2-4 and 3-4. The interaction energy of 2 particles, say particles 1 and 2 in the above list, is:

$$E_{12} = k\frac{q_1 q_2}{d_{12}},$$

where q_1 and q_2 are the charges of these two particles, d_{12} is the distance between particles 1 and 2 and k is a constant, $k = 0.3062$. Similarly, the interaction energy of particles 1 and 3 is:

$$E_{13} = k\frac{q_1 q_3}{d_{13}},$$

etc. The total energy of the system is the sum of all of these individual pairwise interaction energies.

Task

You should write a program that:

- **reads input (the coordinates and charges in the free format as shown above);**
- **calculates the total energy and the total number of pair interactions**
- **outputs the total energy and the total number of pair interactions.**

Please also answer the three questions below:

1. **What is the total energy of the system?**
2. **What is the total number of pair interactions?**

3. How much would the total energy change in percentage if the energy contributions were rounded to the nearest integer number? I.e.

$$E_{12} = Int\left(k\frac{q_1 q_2}{d_{12}}\right).$$

The percentage error in your answer can be found from the formula:

$$\varepsilon = \left|\frac{True\ value - Approximate\ value}{True\ value}\right| \times 100\%$$

Note: Please disregard any use of physical units in this work.

When complete, please submit the source code of your programme and answers to the three questions above to stfcapprentice@ukri.org with the subject line: RSE Assessment Task 1, or provide links to a relevant infrastructure i.e. GitHub/GitLab/etc. where we can examine it.