Molecular dynamics 2015

Exercises 3 to chapter 3: `mdmorse`: Setting initial temperature, building neighbourlist

You can obtain the `mdmorse` code from the course web page:

http://www.acclab.helsinki.fi/~knordlun/moldyn/mdmorse/

1. (8p) Complete the subroutine `SetTemperature()` in `physical.f90/.c` in the code `mdmorse`. This also requires completing the subroutine generating Gaussian random numbers. You may use your solutions of the previous excercises as help.

Check your code by compiling and running `mdmorse`. The routine `GetTemperature()` (which is already provided) should return about twice the input value `initialT`.

2. (12 p) Complete the subroutine `UpdateNeighbourlist()` in `neighbourlist.f90/.c` in `mdmorse`. The subroutine should generate a Verlet neighbour list taking account of the periodic boundary conditions. You do not need to use a linked list.

Hint: when the subroutine in the end outputs the number of neighbours, the answer should be 176.00 with the input files provided in the program distribution.

When coding keep the subroutine parameters as they are given. This makes it easy (for the lecturer) to test them in the original code.

Return the source files `physical.f90/.c` and `neighbourlist.f90/.c`. and the relevant parts of the output (standard output).

When returning subroutines to the code for the exercises, the minimum requirement is that each subroutine returned compiles on a standard Unix/Linux system with

```
gfortran -c filename.f90,
```

or in `C`

```
cc -c filename.c
```

Subroutines which do not compile, give 0 p.