Assignment 1

Problem 1

Two XYZ files are provided in ∼/gianluca/assignment1/:

- `molecule1.xyz`
- `molecule2.xyz`

Note: The first line of an XYZ file contains the number of atoms, the second line is a comment, and subsequent lines contain the Cartesian positions of the atoms, one atom per line: `Element x y z`.

(a) In your personal course directory on the Linux machine, create a subdirectory `assignment1`. Copy the two files from ∼/gianluca/assignment1/ into your `assignment1` folder.

(b) Extract the number of atoms for each XYZ file without opening the files with a text editor. Report the number of atoms in a text file (e.g. `assignment1.txt`) with two lines (for this task you can use the text editor `vim`):

```
molecule1.xyz: <N1> atoms
molecule2.xyz: <N2> atoms
```

(c) Extract only the nitrogen atoms (lines starting with "N") from molecule1 and save them to a file.

(d) Use `vimdiff` to compare `molecule1.xyz` and `molecule2.xyz`. Briefly describe the differences you observe (e.g., atom counts, elements, coordinates).

Problem 2

(a) For each Fortran code below, identify if there is a syntax error.

```
program p
   integer :: x
   x = 2
   if (x > ) then
      write(*,*) 'ok'
   end if
end program p
```

```
program p
   integer :: x, y
   x = 2
   y = 3+ * x
   write(*,*) y
end program p
```

```
program p
   implicit none
   integer :: x
   x = 2
   write(*,*) x
end program p
```

(b) Write a Fortran program that declares a character variable for your name, assigns your name to it, and prints a greeting that includes `Hello World, my name is` followed by your name.

Hint: Use the following statements, replacing `yourname` with your name:

```
character(len=40) :: name  ! variable declaration
name = 'yourname'          ! variable assignment
write(*,*) 'Hello World, my name is ', name  ! printing
```

(c) Compile and run your program from part (b). Check that the output includes the greeting and your name.

(d) Identify the different sections of a Fortran program in the code from the previous question: declaration section, execution section, termination section.