

## 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`.

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

- Extract only the nitrogen atoms (lines starting with “N”) from `molecule1` and save them to a file.
- Use `vimdiff` to compare `molecule1.xyz` and `molecule2.xyz`. Briefly describe the differences you observe (e.g., atom counts, elements, coordinates).

### Problem 2

- For each code snippet below, identify whether the error is a syntax or semantic error (or there is no error). Briefly justify your choice.

```
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
  real :: g, S, q
  g = 0.0
  S = 25.0
```

```

      q = S/g
      write(*,*) q
end program p

```

- (b) Write a Fortran program that declares a character variable for your name, assigns your name to the variable, prints the message "Hello World, my name is [your name]!".

*Hint:* Use the following statements:

```

      character(len=20) :: name      ! variable declaration
      name = "Student"              ! variable assignment
      write(*,*) 'My name is ', name ! printing

```

- (c) Compile and run the code from the previous question.
- (d) Identify the different sections of a Fortran program in the code from the previous question: Declaration section, Execution section, Termination section.