



Input/output and Arithmetic Operations

1. Let's write our first program,

PROGRAM PROJEC

```
*****  
****
```

```
* This program calculates the velocity and height of a projectile  
*
```

```
* given its initial height, initial velocity, and constant      *  
* acceleration. Variables used are:                               *
```

```
* HGHT0   : initial height                                       *
```

```
* HGHT    : height at any time                                   *
```

```
* VELOC0   : initial vertical velocity                           *
```

```
* VELOC    : vertical velocity at any time                       *
```

```
* ACCEL    : vertical acceleration                               *
```

```
* TIME     : time elapsed since projectile was launched          *
```

```
*                                                    *
```

```
* Input:  HGHT0, VELOC0, TIME                                    *
```

```
* Output: VELOC, HGHT                                           *
```

```
*****  
****
```

```
REAL HGHT0, HGHT, VELOC0, VELOC, ACCEL, TIME
```

```
ACCEL = -9.807
```

```
PRINT *, 'ENTER THE INITIAL HEIGHT AND VELOCITY:'
```

```
READ *, HGHT0, VELOC0
```

```
PRINT *, 'ENTER TIME AT WHICH TO CALCULATE HEIGHT AND
```

```

VELOCITY:
  READ *, TIME
  HGHT = 0.5 * ACCEL * TIME ** 2 + VELOC0 * TIME + HGHT0
  VELOC = ACCEL * TIME + VELOC0
  PRINT *, 'AT TIME ', TIME, ' THE VERTICAL VELOCITY IS ',
VELOC
  PRINT *, 'AND THE HEIGHT IS ', HGHT
  END

```

2. Write a program which will convert a temperature of C degrees on the Celsius scale to the corresponding Fahrenheit temperature and display the Fahrenheit temperature. The two scale are related by the following equation:

$$\text{degF} = (9/5) * \text{degC} + 32$$

3. Write a program which writes out the square root of every whole number from 1 to 5. Check it to make sure it runs correctly.
4. Devise a program that takes in three numbers from the keyboard, calls them **a**, **b** and **c**, calculates the equation below and prints the result.

$$\sqrt{b^2 - 4ac}$$

The program will fail when you run it if your values of **a**, **b** and **c** are such that **b²** is less than **4ac**; the computer will not square root a negative number.

5. The Quadratic equation

It's time to write a proper program. Write a program that accepts **a**, **b** and **c** from the keyboard and finds the roots of the quadratic equation:

$$ax^2 + bx + c = 0$$

[When writing even a short program like this, it is valuable to plan first on paper the steps the program must accomplish. For example, in this problem the steps might be: (a) get values of **a**, **b** and **c**; (b) calculate and print the first root; (c) calculate and print the second root; (d) stop. This logical approach improves the chances the program will work correctly.]

Try running your program using **a=2**, **b=5**, **c=2**; then try **a=2**, **b=5**, **c=5**. This second set of coefficients should make your program fail, since the program should then try to square root a negative number - we shall see how to circumvent this difficulty shortly.

Loop programming

1. Temperature conversion

Write a program using a loop which gives a Celsius to Fahrenheit conversion table in units steps from 0°C to 100°C. (To get degrees °F, multiply °C by 9/5, then add 32; to check your result, note that water freezes at 32°F and boils at 212°F.)

2. Range of real variables stored by FORTRAN programs

Write a simple program to find approximately the largest value that can be stored in a real variable. (You might, for example, repeatedly multiply a variable the power of 2 within a loop,

printing the new value on the terminal, until the computer gives up).

3. Range of integer variables stored by FORTRAN programs

Rewrite the above simple program to find approximately the largest value that can be stored in an integer variables.

Arrays

1. Write a program to read some numbers from the terminal and store them in an array. Print out the array to check they were entered correctly. (You must specify the maximum size of the array, since the F77 compiler needs to do know how much memory to allocate to the program).
2. Modify this program to write out the numbers in reverse order.

Checking variables

1. Write a program which takes in a number from the keyboard and checks its size. If the number is less than 100, the program should print on screen "That is small", and if greater than or equal to 100 print something else appropriate. Enclose the code in a loop, so you can enter several numbers one after another.
2. Reconsider the quadratic equation program and use an IF THEN statement to return a message that the discriminant is negative and therefore there are no real roots.

3. Using the last array exercise program and modify it such that it sorts the numbers using the *bubble sort method* . You should end up with the smallest at the beginning of the list , the largest at the end.

The *bubble sort method* - compare the first and second values switch them if they are out of order. The second and third are treated in the same way, and so on. Until a complete pass of the numbers has been done. The numbers are not yet sorted so start another pass. The number of passes requires to ensure sorting will be one less than the number of numbers to be sorted.

Subprograms and Functions

In this exercise we shall calculate the radial distribution function (RDF) for 1s, 2s and 2p orbitals, and then normalize the result so the maximum value of each RDF is one. The RDF is $4\pi r^2$ times the square of the wavefunction. The wavefunctions themselves are given by:

- $1s = e^{-r/2}$
- $2s = 32^{-1/2} (2 - r) e^{-r/2}$
- $2p = 972^{-1/2} (6 - 6r + r^2) e^{-r/2}$

We can divide the problem into a number of distinct steps:

- find out for which orbital calculations are required
- calculate the RDF for an orbital
- scale the calculated values

More Orbital calculations.

Recall a copy of the above exercise and make suitable additions to include the 3p and 3d orbitals.

- $3p = 648^{-1/2} (4r - r^2) e^{-r/2}$
- $3d = 2592^{-1/2} r^2 e^{-r/2}$

