PH502: Scientific Programming Concepts

Irish Centre for High End Computing (ICHEC)

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Overview

- In this lecture we will cover basic aspects of a computer program.
- All aspects of the computers operation, from monitoring the keyboards to graphical windows, are handled by programs.
- In this series we will be concerned with programs for scientific applications written in either C or FORTRAN.

Imperative Programming Paradigm

Knowledge:

- Declarative: Describes properties of things.

$$\sqrt{x} \text{ is } y \text{ such that } y \geq 0 \text{ and } y^2 = x$$

- Imperative: Describes how to do things.
  1. Start with a guess: G.
  2. If $G * G$ is close enough to x, then G is a good approximation of $\sqrt{x}$. Stop.
  3. Else, create a new guess by averaging G and x/G. I.e, $G_{new} = \frac{G+x/G}{2}$.
  4. Using this new guess, go back to Step 2.

Programming Languages

Program is a representation of a set of instructions.

- Low level - High level
- General - Targeted
- Interpreted - Compiled

Syntax $\approx$ Symbolic representation, Legal expression
Semantic $\approx$ Meaning

Two programs written in different languages could do the same thing (semantics) but the symbols used to write the program would be different (syntax).

Basic Program Layout

```
Main

   declare variables

   initialise variables or load initial state

   command to modify store /* O_1 */

   command to modify store /* O_2 */

   ...

   command to modify store /* O_n */

   save final state to disk as required
end
```