PROGRAMMING FOR COMPUTATIONAL CHEMISTRY

Data

Emanuele Coccia

Dipartimento di Scienze Chimiche e Farmaceutiche

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- Subroutine/function and data are distinct entities
- Procedural programming

Practical example

Given two integers n1 and n2, both read from standard input, we want to sum them into a variable total, then printed on the screen (standard output) (add.f90)

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- KB, MB, GB, TB etc.

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- character*p: string of alphanumeric character, with length p

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  1. set of values (domain)
  2. set of operations

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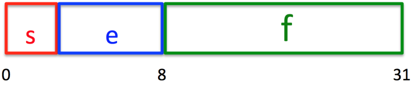
- Floating point numbers used to approximate real numbers
- Scientific notation in base 2

Floating point arithmetics

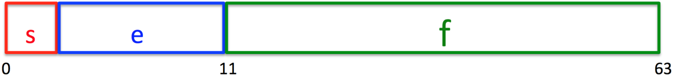
- Single precision (real*4): 32 bits, from $\sim 1.175 * 10^{-38}$ to $\sim 3.403 * 10^{+38}$
- Double precision (real*8): 64 bits, from $\sim 2.225 * 10^{-308}$ to $\sim 1.798 * 10^{+308}$

$$\text{floating point} = (-1)^{s} * f * 2^{e}$$

Single precision



Double precision



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- Finite number of significant digits
- Finite range
- Systematic error in representing real numbers (round-off error)

Base 2

$$101.01 = 1 \times 2^2 + 0 \times 2^1 + 1 \times 2^0 + 0 \times 2^{-1} + 1 \times 2^{-2} = 5.25$$

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$$\begin{aligned}
101.01 &= 1 \times 2^2 + 0 \times 2^1 + 1 \times 2^0 + 0 \times 2^{-1} + 1 \times 2^{-2} = 5.25 \\
0.0101 &= 0 \times 2^0 + 0 \times 2^{-1} + 1 \times 2^{-2} + 0 \times 2^{-3} + 1 \times 2^{-4} \\
&= 1./4. + 1./16. = 0.3125
\end{aligned}$$

Practical examples

- Rewrite add.f90 with real and double precision numbers