CS601: Software Development for Scientific Computing

Autumn 2024

Week2: Real numbers and their program representation

Recap: Scientific Computing

Physical process

↓

Mathematical model

↓

Algorithm

↓

Software program

↓

Simulation results

Recap: Toward Scientific Software

- Necessary Skills:
  1. Understanding the mathematical problem
  2. Understanding numerics
  3. Designing algorithms and data structures
  4. Selecting language and using libraries and tools
  5. Verify the correctness of the results
  6. Quick learning of new programming languages

Recap: Computational Thinking

- Abstractions
  - Our "mental" tools
  - Includes: <u>choosing right abstractions</u>, operating at multiple <u>layers</u> of abstractions, and defining <u>relationships</u> among layers
- Automation
  - Our "metal" tools that <u>amplify</u> the power of "mental" tools
  - Is mechanizing our abstractions, layers, and relationships
    - Need precise and exact notations / models for the "computer" below ("computer" can be human or machine)
- *Computing is the automation of our abstractions*

Scientific Software - Motifs

noun

1. a decorative image or design, especially a repeated one forming a pattern.
   "the colourful hand-painted motifs which adorn narrowboats"

   Similar: design | pattern | decoration | figure | shape | logo | monogram

2. a dominant or recurring idea in an artistic work.
   "superstition is a recurring motif in the book"

1. Finite State Machines
2. Combinatorial
3. Graph Traversal
4. Structured Grid
5. Dense Matrix
6. Sparse Matrix
7. FFT
8. Dynamic Programming
9. N-Body (/ particle)
10. MapReduce
11. Backtrack / B&B
12. Graphical Models
13. Unstructured Grid

Real Numbers $\mathbb{R}$

- Most scientific software deal with Real numbers. Our toy code dealt with Reals
  - Numerical software is scientific software dealing with Real numbers
- Real numbers include rational numbers (integers and fractions), irrational numbers (pi etc.)
- Used to represent values of continuous quantity such as time, mass, velocity, height, density etc.
  - Infinitely many values possible
  - But computers have limited memory. So, have to use approximations.

Representing Real Numbers

- Real numbers are stored as *floating point numbers*
  (floating point system is a scheme to represent real numbers)
- E.g. floating point numbers:
  - $\pi = 3.14159,$
  - $6.03*10^{23}$
  - $1.60217733*10^{-19}$

General format: $\pm x \times b^{e}$

exponent

mantissa

(number ranges from:
1 to b   OR   1/b to 1

If 1 to b then
$x_0.x_1x_2x_3 \ldots x_{m-1}$)

base

(e.g. base 10, 8, 2, 16)

3-Digit Decimal Representation

- Suppose base, b=10 and
- $x = \pm d_0 . d_1 d_2 \times 10^e$ where $\begin{cases} 1 \leq d_0 \leq 9, \\ 0 \leq d_1, d_2 \leq 9, \\ {\scriptstyle -9 \leq e \leq 9} \end{cases}$
- precision = length of mantissa
  - What is the precision here?
- Exercise: What is the smallest positive number?
- Exercise: What is the largest positive number?
- Exercise: How many numbers can be represented in this format?
- Exercise: When is this representation not enough?

Floating Point System - Terminology

- **Precision (p)** - Length of mantissa
  - E.g. p=3 in 1.00×10^{-1}
- **Unit roundoff (u)** – smallest positive number where the *computed* value of 1+u is different from 1
  - E.g.   suppose p=4 and we wish to compute 1.0000+ 0.0001=1.0001
  - But we can't store the exact result (since p=4). We end up storing 1.000.
  - So, computed result of 1+u is same as 1
  - Suppose we tried adding 0.0005 instead. 1.0000+0.0005=1.0005 Now, round this: 1.001

  $\Rightarrow$ **u =0.0005**
- **Machine epsilon (ϵ_{mach})** – smallest a-1, where a is the smallest representable number greater than 1
  - E.g. consider 1.001 – 1.000 = 0.001.

  $\Rightarrow$ **usually ϵ_{mach} = 2 * u**

Exercise: 3-Digit Binary Representation

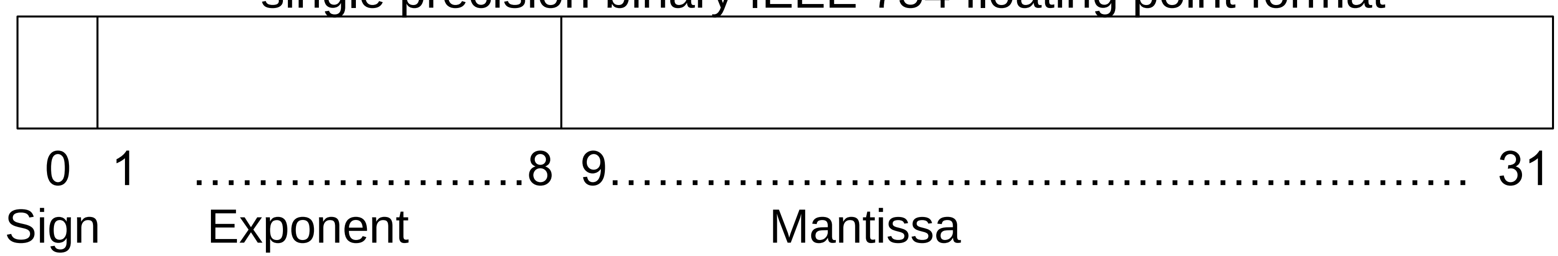
- Suppose base, b=2 and
- $x = \pm b_0.b_1 b_2 \times 2^E$,where $\begin{cases} 1 \leq b_0 \leq 1, 0\ iff\ b_1, b_2 = 0 \\ 0 \leq b_1, b_2 \leq 1, \\ -1 \leq E \leq 1 \end{cases}$
- What is the precision?
- What is the unit roundoff?
- What is the machine epsilon?
- What are the range of numbers that can be represented?

IEEE 754 Floating Point System

- Prescribes single, double, and extended precision formats

Precision	**u**	**Total bits used (sign, exponent, mantissa)**
Single	$6x10^{-8}$	32 (1, 8, 23)
Double	$2x10^{-16}$	64 (1, 11, 52)
Extended	$5x10^{-20}$	80 (1, 15, 64)

single precision binary IEEE 754 floating point format



IEEE 754 Floating Point Arithmetic

double precision binary IEEE 754 floating point format

Sign	Exponent	Mantissa
0	1……………………..11	1………………………………………….52

- if exponent bits e_1-e_{11} are not all 1s or 0s, then the *normalized* number

$$n = \pm(1.m_1 m_2 .. m_{52})_2 \times 2^{(e_1 e_2 .. e_{11})_2 - 1023}$$

- **Machine epsilon** is the gap between 1 and the next largest floating point number. $2^{-52} \approx 10^{-16}$ for double.
- Exercise: What is minimum positive *normalized* double number?
- Exercise: What is maximum positive *normalized* double number?