ESC201: Simulations in the Natural Sciences

Monday, 18 September 2023 11:22

https://www.ics.uzh.ch/~stadel

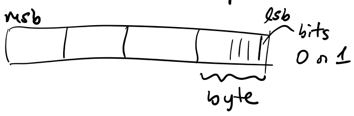
Teaching Assistants: **Stefan Schafroth**
Grading: 40% Assignments, **60% Final Oral Exam**

Language: Python3

Plan for the Course:
- Numbers and Root Finding
- Newton's method and Kepler's Equation
- Population Growth, Chaos and Fractals
- ODEs (ordinary differential equations): Predator-Prey behaviour
- Symplectic Integration
- Solar System Simulation
- PDEs (partial differential equations)
- Elliptic PDEs: Laplace Equation
- Interpolation on a grid: Simulating Electrons
- **Design Prize!**
- Parabolic PDEs: Diffusion and Stability
- Hyperbolic PDEs: Upwind Finite Difference
- Finite Volume Methods
- 2-D advection: Corner Transport Upwind Method
- 1-D Hydrodynamics (2-D would be awesome!)
- **Oral Exam** (in last week of the Semester)

How are numbers represented on the Computer

• Integers : 32-bits



$\emptyset$: all bits $\emptyset$ ✓

+1: 0000 ······ 0001 — 2's complement representation

−1: 1111 ······ 1111

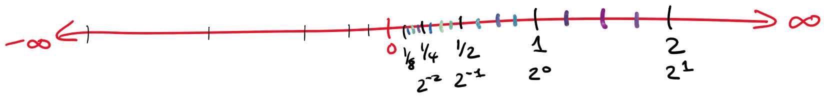
Most negative number:

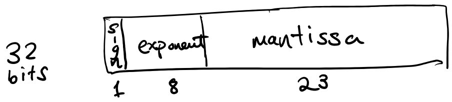
1 000 ····· 0000 $= -2^{31}$

Most positive number:

0 111 ···· 1111 $= +2^{31} - 1$

Floating Point numbers ≠ Real numbers





"float"

STANDARD IEEE-754

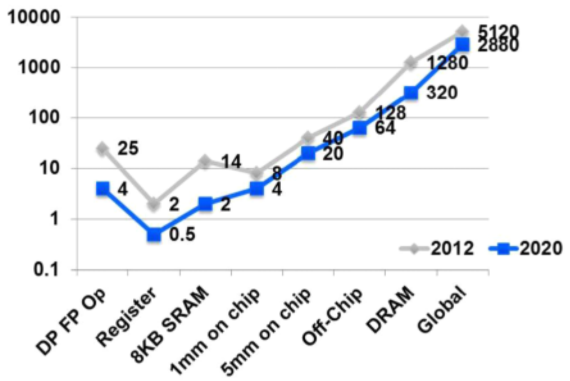


Figure 5: *Energy cost, in picojoules (pJ) per 64-bit floating-point operation, for various common operations within a computer. The upper (gray) line characterizes energy cost estimates in 2012 technology, and the lower (blue) line projects costs in 2020. Note that the double-precision floating-point arithmetic (DP FP Op) energy cost is comparable to that for moving the same data 1mm–5mm on chip; that cost is dwarfed by the cost of any movement of this same data off chip.*

Rounding: 1,6|5 $\Rightarrow$ 1,~~7~~ 1.6

1,7|5 $\Rightarrow$ 1.8

9
8
7
6
5 ↑ biased

Rounding:

$1{,}6|5 \Rightarrow \cancel{1{,}7}$ 1.6

$1.7|5 \Rightarrow 1.8$

Round to nearest even

$1.6 \,|\, 8\ 7\ 6\ 5\ 4\ 3\ 2\ 1$ biased

$1.0 1 | 1\ 0$

$\pm$ infinity, ± 0, NAN

$0/0$

```
r2 = x*x + y*y + z*z;
assert (r2 >= 0);
r = sqrt(r2);
```

FORMULAS (nice)

$$ax^2 + bx + c = 0$$ solve for x

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \quad \boxed{A}$$

$$x = \frac{2c}{-b \pm \sqrt{b^2 - 4ac}} \quad \boxed{B}$$

NEVER use these

a and/or c can be small

$$q = -\frac{1}{2}\left[b + \underset{+1,-1}{\operatorname{sign}(b)} \cdot \sqrt{b^2 - 4ac}\right]$$

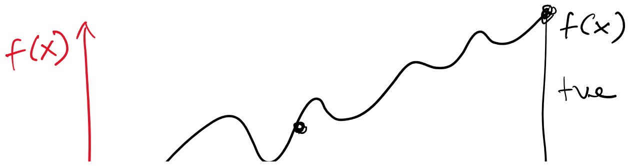
$$x_1 = \frac{q}{a} \qquad x_2 = \frac{c}{q}$$

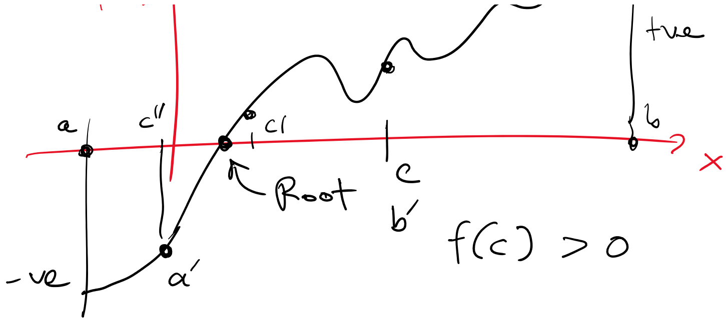
$$ax^3 + bx^2 + cx + d = 0 \quad \checkmark$$

$$ax^4 + bx^3 + cx^2 + dx + e = 0 \quad \checkmark$$

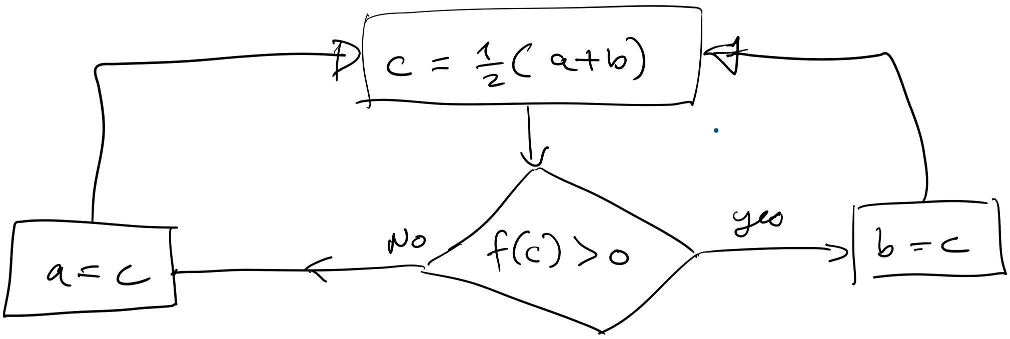
No formula – no problem! $f(x) = 0$

$x^x = 100$? $\rightarrow f(x) = x^x - 100$





Bisection Method



#1 Never stops !?!

#2 More than one root!

#3 Continuous — don't worry...

#4 $f(a) > f(b)$!? ⇐ ✓

$x^x - 100 = 0$ Solve