ESC 201: Simulations in the Natural Sciences

Monday, 19 September 2022 11:01

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

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Grading: 40% Assignments, **60% Final Oral Exam**

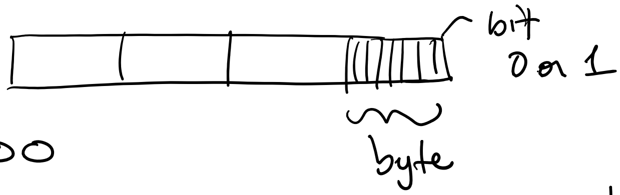
Language: Python3

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 numbers are represented on the computer?

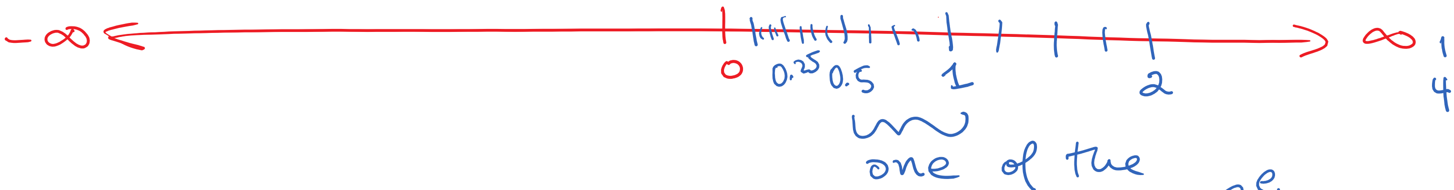
- Integers: 32-bits



∅: 0000 ····· 0000
+1: 0000 ···· 0001
−1: 1111 ···· 1111 — 2's complement 0 − 1

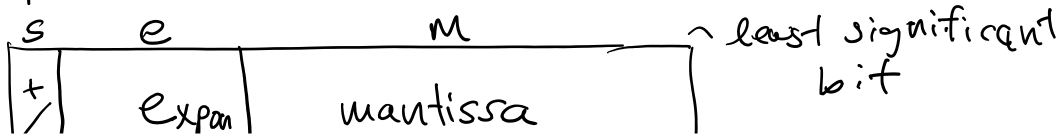
Most negative number:
10000 ···· 0000 $= -2^{31}$
Most positive number:
0111 ····· 1111 $= +2^{31} - 1$

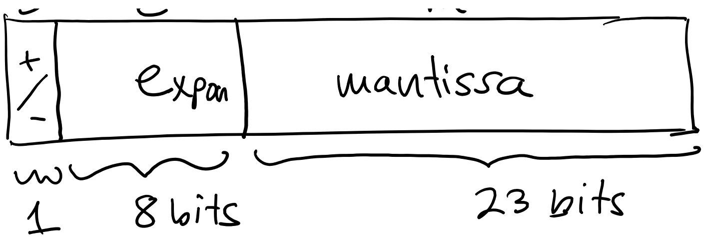
Floating Point numbers ≠ Real numbers!



2^e

IEEE-754 Standard





$\pm 1.23456 \times 10^{12}$ Scientific Notation

7.8912×10^{8} normalized

Binary $\boxed{1.}001011\ldots \times 2^{101}$

$\varnothing$: 00000000000 000

$$s \times 1.M \times 2^{E-127}$$

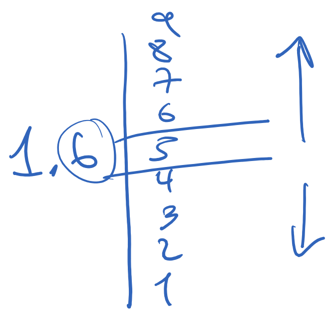
double

Energy? ⊕ 5 picojoules
⊛ 4

= ~1000 picojoules

1.6|5 ⇒ 1.6 Round to nearest

1.7|5 ⇒ 1.8



± infinity, ±0, NAN

0/0 = ? NAN

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

FORMULAS : (nice)

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

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

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

When either a and/or c is small

$-b \pm \sqrt{b^2 - 4ac}$ — $4ac$ small

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

sign(b): +1, -1

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

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cubic equations $ax^3 + bx^2 + cx + d = 0$

$ax^4 + \dots = 0$

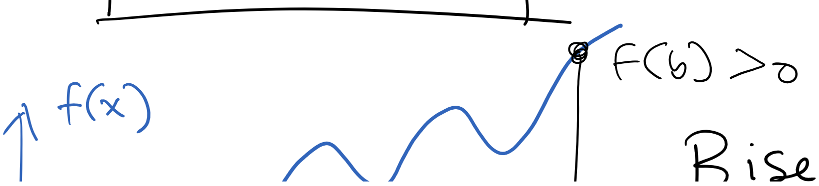
~~$ax^5 + \dots = 0$~~

$x^x = 100 \Rightarrow x^x - 100 = 0$

No Formula → No problem

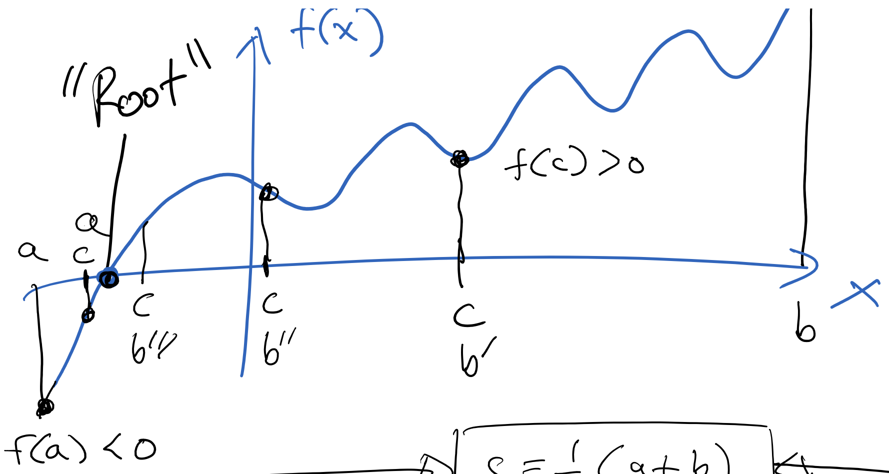
$$\boxed{f(x) = 0}$$

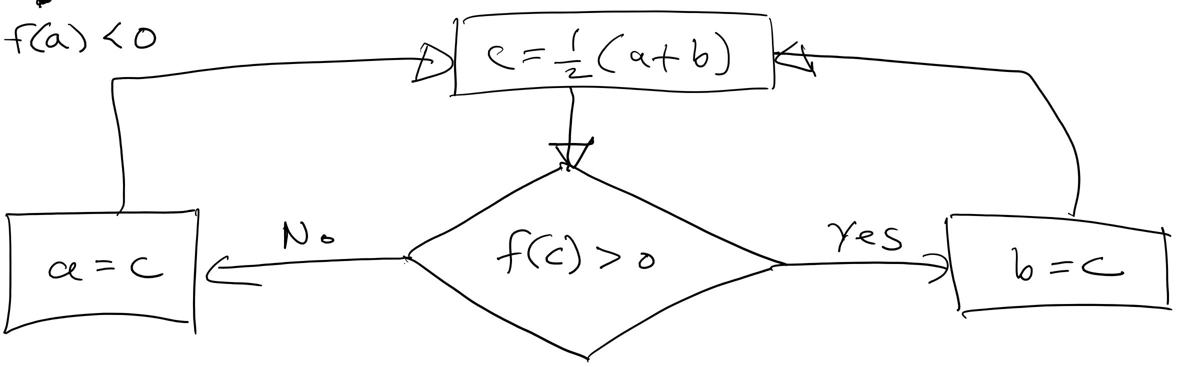
"Root"



Bisection

Bisection Method





Infinite Loop!
Break out of this?

$|a-b| < \varepsilon_{absolute}$ (e.g. millikelvin)

or

$$\frac{|a-b|}{|c|} \leq \varepsilon_{relative}$$

Assumed f(a) is negative and that f(b) is positive

what if it is the opposite?

$f(x) = x^x - 100$ and Quadratic (a, b, c)

Bad: $A(x) = \dfrac{x-1}{e^{x-1}-1}$ $\quad A(1.0) = 1.0$!