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生態模擬:以C語言為例

- How to solve algebraic equation and how to reduce numerical errors
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11.1 Numerical errors (0): How to use complex number

You can use complex number including the library <complex.h>

Just try to compile and execute 'complex_test0.c'

```
#include <stdio.h>
#include <math.h>
#include <stdlib.h>
#include <time.h>
#include <complex.h>
int main(void){
  double complex x;
  x = 3.0 + 1*4.0;
   printf("real=%lf\timg=%lf\tabsolute value = %lf\n", creal(x), cimag(x), cabs(x));
                                                 Real part c
   return 0;
                                                            Imaginary
                                                                       length of
```

Functions in real sqrt(x), exp(x), fabs(x)... \leftrightarrow csqrt(x), cexp(x), cabs(x)...

11.2 Numerical errors (0): IEEE 754

IEEE 754: Standard for Binary Floating-Point Arithmetic, which is organized the **I**nstitute of **E**lectrical and **E**lectronics **E**ngineers, Inc.) (I triple E).

We need many roles for arithmetic calculations in computer for keeping the quality of calculation with controlling errors.

IEEE 754 is adopted as default specification in some language (e.g. C#, Java) but not in C language. However, it is recommended to follow IEEE754 even in C language.

For example, IEEE 754 determines the specification of **float** and **double**.

→Topic 1

Also, it determines the roles of **rounding algorithms** (c.f. 四舍五入)

→Topic 2

11.2 Numerical errors (0): IEEE 754, floating point number

What is floating point number?

In the decimal system (十進位)

fraction
$$-10.34 = -1.034 \times 10^{1}$$
sign
$$-10.34 = -1.034 \times 10^{1}$$
base
$$-10.34 = -1.034 \times 10^{1}$$

$$-10.34 = -1.034 \times 10^{1}$$

In the binary system (二進位)

$$-2.5 = -(1x2^{1} + 0x2^{0} + 1x2^{-1}) = -10.1$$

$$-10.1 = -1.01 \times 2^{1}$$

11.2 Numerical errors (0): IEEE 754, floating point number

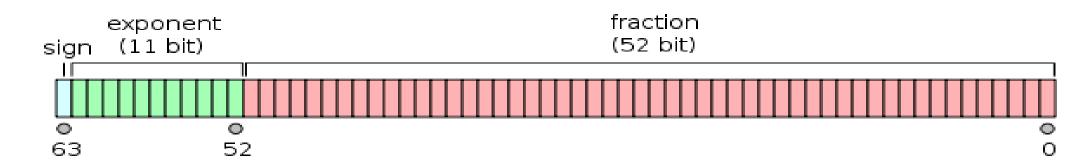
"double" is defined in IEEE 754

In the binary system (二進位)

$$-2.5 = -(1x2^{1} + 0x2^{0} + 1x2^{-1}) = -10.1$$

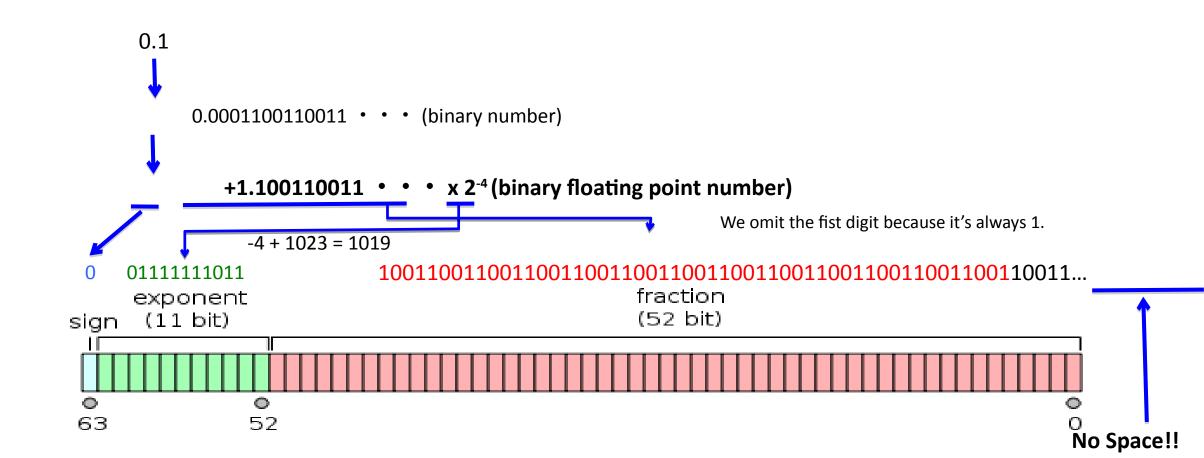
$$-10.1 = -1.01 \times 2^{1}$$

Type Double (64bit)



What is the source of rounding 'error'??

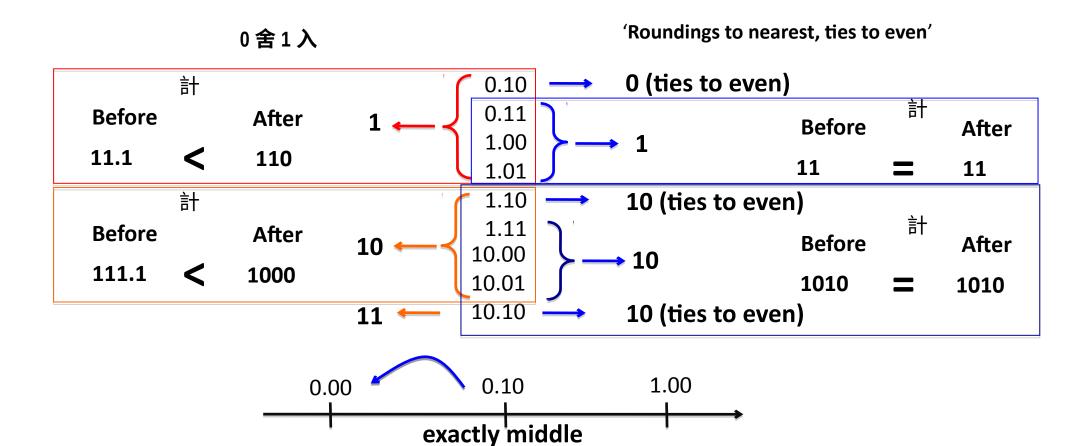
Consider converting 0.1 (in decimal system) to a binary number and to floating point number. We need one digit for 0.1 in decimal system, but in the binary system we need infinite number of digits: 0.1 = 0.0001100110011 • • • . . However, we can use only 52 bit of memory to stock the fraction part of this number.



We need common rules on how to round numbers.

One of common rules in IEEE 754 is 'Roundings to nearest, ties to even'

Consider a simple hypothetical trial to round two digits of binary for understanding the difference bet. the **roundings** to nearest and simple 0 舍 1 入



Common rules in IEEE 754 is not included in mathematical library <math.h>.

One of alternative libraries is:

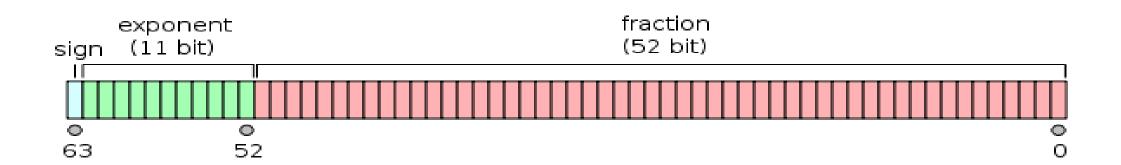
CRlibm Correctly Rounded mathematical library

http://lipforge.ens-lyon.fr/www/crlibm/

However, I would not say Crlibm is always better than libm...

cf) intel C compiler (icc) also includes specific math library

Do you think this type of error is critical?



11.3 Numerical errors (1): what is the loss of significant digits?

Let's consider a simple example, trying to calculate the following when the significant digit number = 8 (let's think only in the decimal system).

$$\sqrt{1001} - \sqrt{999}$$

Round-off errors occur in the final digit.

$$\sqrt{1001} = 31.6385840 \dots \approx 31.638584$$
 (error: 1.2 x 10⁻⁷ %

$$\sqrt{999} = 31.6069612 \cdots \approx 31.606961$$
 (error: 8.2 x 10⁻⁷ %)

$$\sqrt{1001}$$
 - $\sqrt{999} \approx 31.638584$ - 31.606961

$$= 0.031623 = 3.1623000 e - 2$$
 \leftarrow should be 3.1622781e-2

error: 6.9 x 10⁻⁴ %!!

Round-off error in the final digit.

Round-off error jumps up to 5th digit!!

→ loss of significant digits!!

Numerical errors (2): what happens in logistic map? **11.4**

Let's consider a simulation of logistic map, using x as float or y as double (see logistic error.c).

float
$$x = 0.1$$
;
double $y = 0.1$;

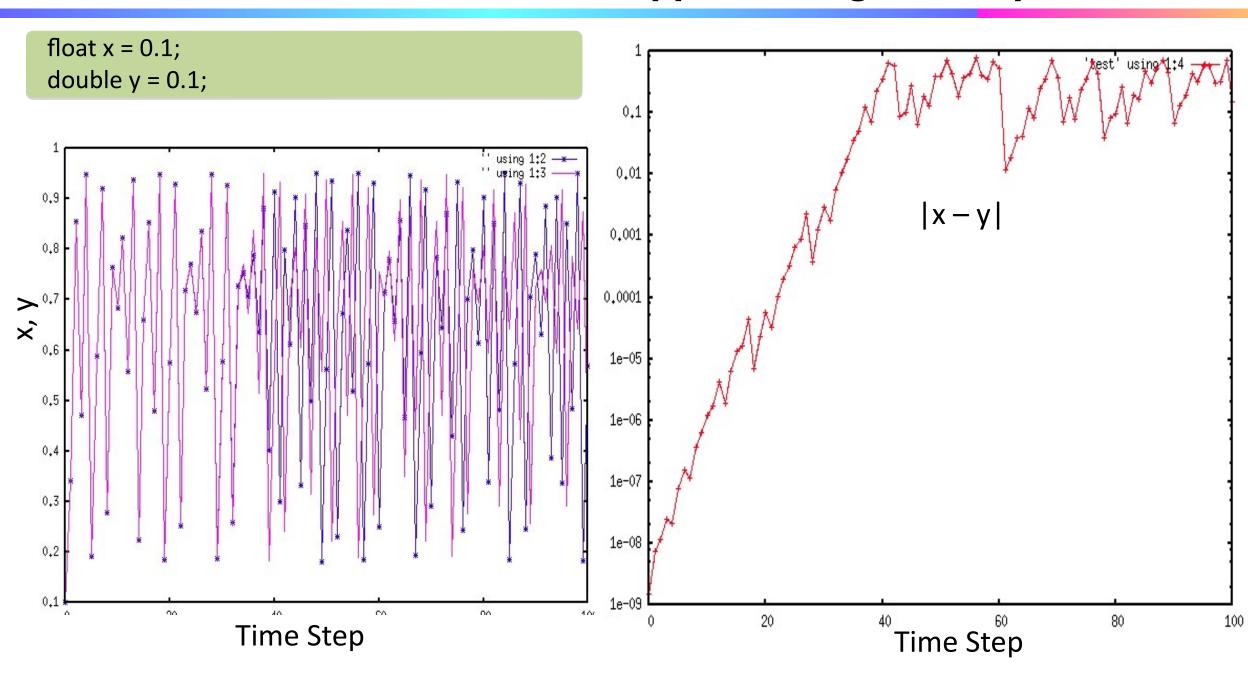
$$\mathbf{x}_{t+1} = 3.8 \cdot \mathbf{x}_t \cdot (1.0 - \mathbf{x}_t)$$

$$x_{t+1} = 3.8 \cdot x_t \cdot (1.0 - x_t)$$

 $y_{t+1} = 3.8 \cdot y_t \cdot (1.0 - y_t)$

Loss of significant digits occurs In this subtraction.

11.4 Numerical errors (2): what happens in logistic map?



11.4 Numerical errors (2): what happens in logistic map?

Suggestions from logistic map:

The source of the cancellation of significant digit is the rounding error.

Therefore, we can suppress this error by using double instead of float.

 \rightarrow In some computer systems, you can further increase the memory size for floating point numbers.

Is this unique solution?

→NO!!

First, we need to go back to...

We can reduce the error by avoiding the subtraction between similar size of number!!

$$\sqrt{1001} - \sqrt{999} = \frac{(\sqrt{1001} - \sqrt{999})(\sqrt{1001} + \sqrt{999})}{(\sqrt{1001} + \sqrt{999})}$$

$$= \frac{2}{(\sqrt{1001} + \sqrt{999})} \approx \frac{2}{31.638684 + 31.606961}$$

$$= \frac{2}{32.245545} \approx 0.031622781 \qquad \text{error: } 1.8 \times 10^{-6} \%!!$$

Then, try to think about the good algorithm for solving quadratic equation.

We have an formula for exact solution!!

$$ax^{2} + bx + c = 0$$

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

But, when $b^2 >> 4ac$

$$-b\pm\sqrt{b^2}-4ac \approx -b\pm|b|$$

...leading to loss of significant digits

Let's assume

$$D = b^2 - 4ac > 0$$

A better formula is:

if
$$(b>0)$$

$$x_{1} = \frac{-b - \sqrt{b^{2} - 4ac}}{2a}$$

else

$$x_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a}$$

$$x_2 = \frac{c}{ax_1}$$

Compare the performance of *quadratic_solver* and *quadratic_bad_solver* in solver_test0.c for following equations.

$$(x-1)(x-5) = 0$$

 $(x-1)(x-1.001) = 0$
 $(x-1.0 \cdot 10^6)(x-1.2345678912345 \cdot 10^{-10}) = 0$

$$x^2 + x + 1 = 0$$

11.6 Further information

Generally, there are gaps between analytical formula and numerical algorithm.

In calculations of floating point number, the following 'associative law' does NOT hold.

$$a + (b + c) = (a + b) + c$$

'Numerical Verification method' to control the worst error size and thus ensure the quality of simulations is a growing field in applied math. With this method, we are able to prove mathematical theorems using computer!! e.g. existence or uniqueness of solution or attractor in ODE/PDE