Numbers representation with computers, errors and uncertainties in computations

M. Peressi - UniTS - Laurea Magistrale in Physics Laboratory of Computational Physics - Unit I - part II

Number representation in a given basis

A real number in basis 10:

$$741.36 = 7 \cdot 10^{2} + 4 \cdot 10^{1} + 1 \cdot 10^{0} + 3 \cdot 10^{-1} + 6 \cdot 10^{-2}$$

If b is the basis, the string: $a_k a_{k-1} a_{k-2} \dots a_0 a_{-1} a_{-2} \dots a_{-k}$

$$a_k a_{k-1} a_{k-2} \dots a_0 a_{-1} a_{-2} \dots a_{-k}$$

represents:
$$\sum_{i=-k}^{k} a_i b^i = a_k b^k + a_{k-1} b^{k-1} + \dots + a_0 b^0 + a_{-1} b^{-1} + \dots + a_{-k} b^{-k}$$

Another example: integer number, basis 2:

$$(1001)_2 = 1 \cdot 2^3 + 0 \cdot 2^2 + 0 \cdot 2^1 + 1 \cdot 2^0 = (9)_{10}$$

Number representation in a computer

- the microscopic unit of memory is the BIT=(0,1)

$$1 \text{ BYTE} = 1B = 8 \text{ BITS}$$

 $1K = 1KB=2^{10}BYTES=1024 BYTES$

- BIT=(0, I) => binary form for number representation
- the representation of a number in a computer is characterized by the numbers of bits used to store it
- fixed point or floating point representation (for integers) (for reals)

Fixed point representation for integers

$$(1001)_2 = 1 \cdot 2^3 + 0 \cdot 2^2 + 0 \cdot 2^1 + 1 \cdot 2^0 = (9)_{10}$$

- With N bits, typically the first one is reserved to the sign: N-I bits available =>

it is possible to represent numbers with <u>absolute</u> value in $[0, 2^{N-1}-1]$

If you try to go beyond: OVERFLOW (i_min_max.f90)

Fixed point representation for integers

On INFIS: the result is $[-2^{31}, 2^{31}-1]$; why?

Floating point representation for real numbers

$$x_{float} = (-1)^s \bullet mantissa \bullet b^{\exp fld - bias}$$

Sign

significant exponent

figures of of the

the number;

number

basis b=2

- Typically: expfld = 8-bit integer (goes from [0,255]) bias = 128 (or 127) => expfld-bias goes from -128 to +127 (or from -127 to +128); 23 bits reserved for the mantissa => tot 32 bits $\frac{mantissa}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_{23} \cdot 2^{-23}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_2 \cdot 2^{-2}}{mantissa} = \frac{m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + ... \cdot m_2 \cdot 2^{-2}}{mantissa} = \frac{m_1$

- precision: 2⁻²³ ~= 6-7 decimal figures
- range : $\sim -10^{-39} 10^{+38}$

examples of floating point representation for real numbers

the smallest: (if mantissa is in the normalized form, i.e., first number =/= 0)

0 1111 1111 1111 1111 1111 1111 1111 $1111 = 2^{128} = 3.4 \times 10^{38}$

single and double precision

For double precision:

```
- Typically: expfld = 11-bit integer (goes from [0,2047]) bias = 1023 => expfld-bias goes from -1023 to +1024; 52 bits reserved for the mantissa => tot 64 bits
```

- precision: 2⁻⁵² ~= 15-16 decimal figures
- range : $\sim -10^{-322} 10^{+308}$

```
If you try to go beyond these limits (see rs(d)_under_over.f90): UNDERFLOW (too small) and OVERFLOW (too large)
```

Roundoff errors

$$7 + 1.0 \times 10^{-9} = ????$$

Single precision representation:

Exponents are different! Make them equal before operating on the mantissas: increase the smallest exponent, but at the same time reduce the corresponding mantissa:

Machine precision

The smallest number that, added to I represented in the machine, does not change it:

$$\varepsilon_m + 1_c = 1_c$$

- $\varepsilon \cong 10^{-7}$ single precision
- $\varepsilon \cong 10^{-16}$ double precision

Note: IT IS NOT the smallest representable number!

See also: intrinsic function epsilon(x)

Source of errors in numerical computing

- Human
- Random (e.g. electrical fluctuations)
- Roundoff
- Truncation

$$2\left(\frac{1}{3}\right) - \frac{2}{3} = 2 \times 0.3333333 - 0.6666667 = -0.0000001 \neq 0.$$

$$e^{x} = \sum_{n=0}^{\infty} \frac{x^{n}}{n!} \cong \sum_{n=0}^{N} \frac{x^{n}}{n!} = e^{x} + E(x, N)$$

Mainly ROUNDOFF,
due to the finite representation of numbers
in a computer

An example of roundoff+truncation Numerical derivatives

Calculate the derivative of:

$$f(x) = sin(x)$$
 in $x = 1$

We call:

$$f_0 = f(x), f_1 = f(x+h), e f_{-1} = f(x-h).$$

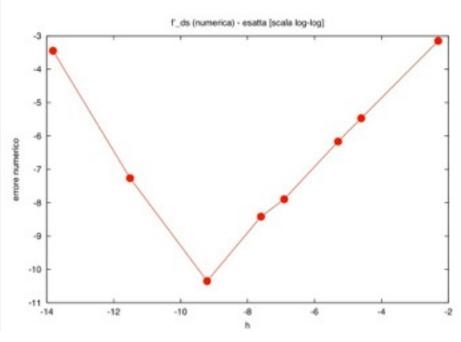
We can use several algorithms:

$$f'(x) \sim \frac{f_1 - f_{-1}}{2h}$$
 $(=f'_{simm})$
 $f'(x) \sim \frac{f_1 - f_0}{h}$ $(=f'_{ds})$
 $f'(x) \sim \frac{f_0 - f_{-1}}{h}$ $(=f'_{sin})$

Make numerical experiments with h and progressively reduce it ...

An example of roundoff+truncation Numerical derivatives

h	f' _{ds}	f'ds-exact	f' _{sin}	f' _{sin} - exact	f' _{simm}	f' _{simm} - exact
0.1	0.497364	-0.042938	0.581441	0.041138	0.539402	-0.000900
0.01	0.536087	-0.004215	0.544497	0.004195	0.540294	-0.000009
0.005	0.538200	-0.002102	0.542398	0.002095	0.540302	0.000000
0.001	0.539930	-0.000372	0.540688	0.000386	0.540323	0.000021
0.0005	0.540081	-0.000221	0.540482	0.000180	0.540310	0.000007
0.0001	0.540334	0.000032	0.540154	-0.000148	0.540384	0.000082
1E-05	0.539602	-0.000701	0.538240	-0.002063	0.540321	0.000019
1E-06	0.508436	-0.031866	0.519472	-0.020830	0.527957	-0.012345

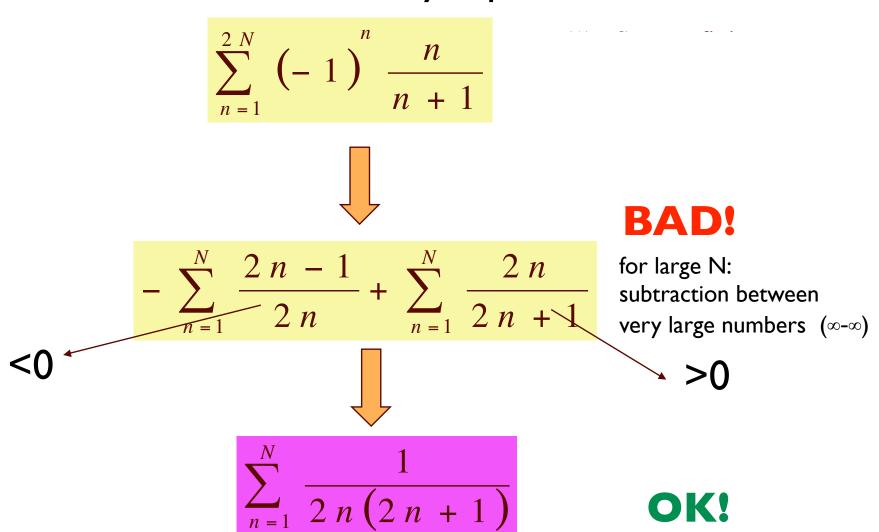


- The symmetric algorithm is the best
- By reducing h down to $\sim 10^{-4}$ the numerical error decreases, but further reduction of h does not improve the result, or better, the result is even worse! Why? **roundoff error**

Other possible sources of errors due to roundoff

- subtraction between very large numbers $(\infty - \infty)$ (see examples: exp-bad.f90)

expressions analytically equivalent can be NOT numerically equivalent!



How does your computer make a calculation?

(remember... this is a common source of HUMAN error in coding)

$$1/2 = ???? 0 !!! WRONG$$

since this operation is done within the INTEGERS

$$1./2 = ??? \quad 0.5 !!! \quad CORRECT$$

since 2 is promoted to REAL and the operation is done within the REALS

Some programs:

in \$/home/peressi/comp-phys/I-basics/f90:

```
deriv.f90; d_strano.f90
exp-good.dp.f90 ; exp-good.f90
i_min_max.f90
rd_under_over.f90 ; rs_under_over.f90
rs_limit.f90 ; rd_limit.f90
strano.f90
test l - subr-funct.f90 ; test 2 - subr-funct.f90
test_factorial.f90
```