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Numbers representation with computers, errors and uncertainties in computations

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

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 BYTE = 1B = 8 BITS

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

- BIT=(0,1) => 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

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

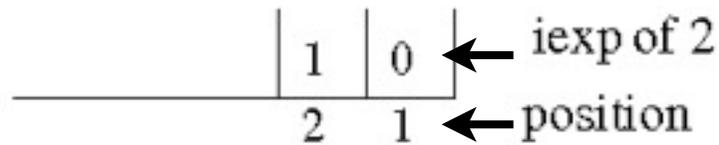
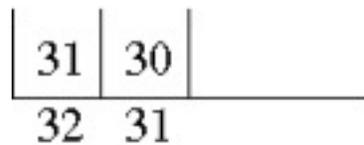
- With **N bits**, typically the first one is reserved to the sign: N-1 bits available =>

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

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

Fixed point representation for integers

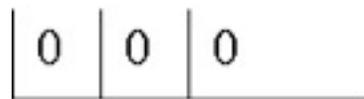
Assume 32 bits available: the result could be $[-2^{31}, 2^{31}-1]$; why?



$$+ (2^{30} + 2^{29} + \dots + 2^0) = 2^{31} - 1$$



$$-2^{31}, \text{ NOT } +2^{31}, \text{ NOT } 0$$



this is 0



$$- (2^{30} + 2^{29} + \dots + 2^0) = -(2^{31} - 1)$$

$$(2^{31} \sim 2 \times 10^9)$$

Floating point representation for real numbers

$$x_{float} = (-1)^s \cdot \underset{\substack{\text{sign} \\ | \\ \text{significant} \\ \text{figures of} \\ \text{the} \\ \text{number}}}{mantissa} \cdot \underset{\substack{\text{exponent} \\ \text{of the} \\ \text{number;} \\ \text{basis } b=2}}{b^{\text{exp fld} - \text{bias}}}$$

- 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

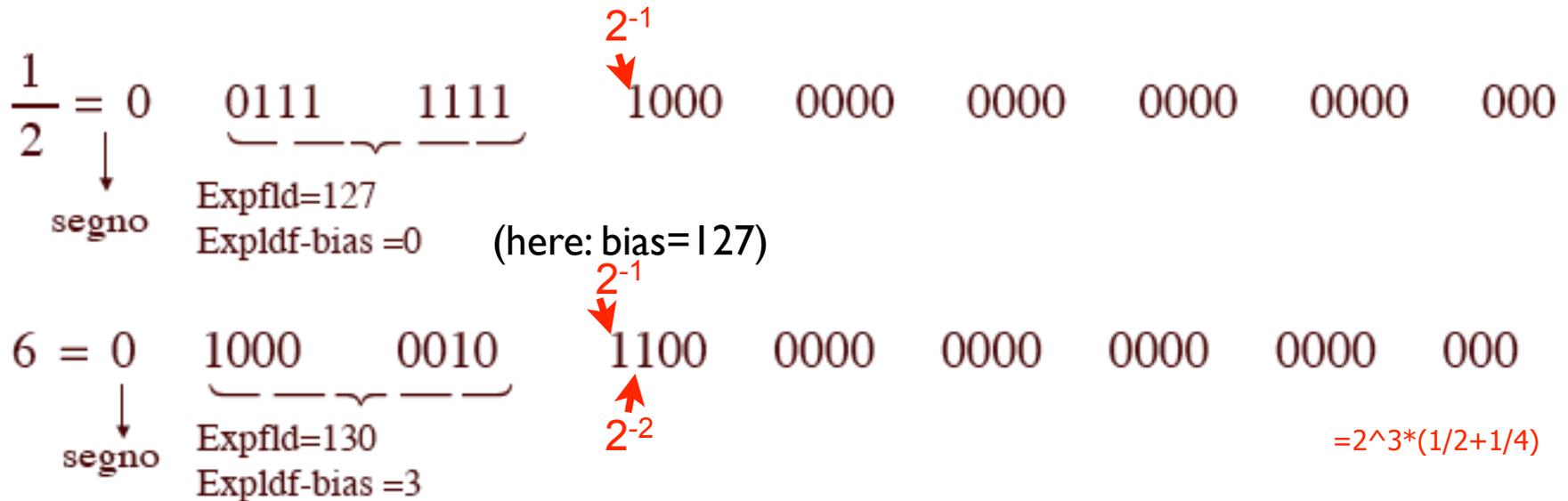
$$mantissa = m_1 \cdot 2^{-1} + m_2 \cdot 2^{-2} + \dots + m_{23} \cdot 2^{-23}$$

(m_1 NOT 0!)

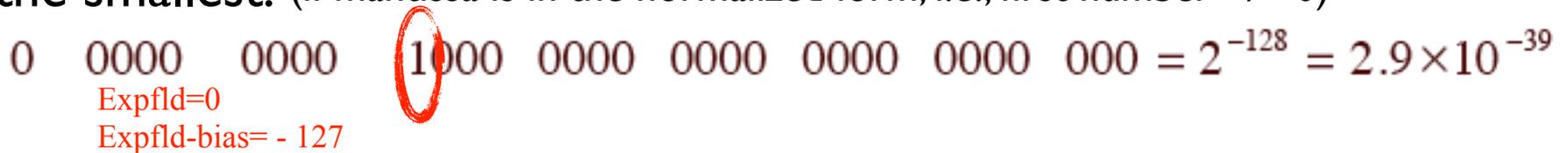
- precision: $2^{-23} \approx$ 6-7 decimal figures

- range : $\sim -10^{-39} - 10^{+38}$

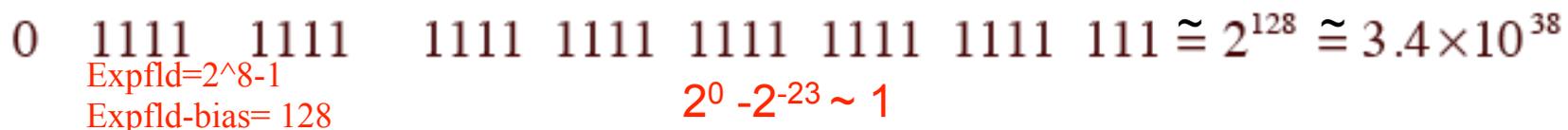
examples of floating point representation for real numbers



the smallest: (if mantissa is in the normalized form, i.e., first number $\neq 0$)



the largest:



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: $2^{-52} \approx 15\text{-}16$ 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:

$$7 = 0 \quad \underline{1000 \quad 0010} \quad 1110 \quad 0000 \quad 0000 \quad 0000 \quad 0000 \quad 000$$

$$10^{-9} = 0 \quad 0110 \quad 0000 \quad 1101 \quad 0110 \quad 1011 \quad 1111 \quad 1001 \quad 010$$

(here: bias=127)

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

	x2 (i.e., +1 in expfield)	:2 (right hand-side shift of the bits)	(bits lost)
$10^{-9} = 0$	0110 0001	0110 1011 0101 1111 1100 101	(0)
$= 0$	0110 0010	0011 0101 1010 1111 1110 010	(10)
.....,			
$= 0$	1000 0010	0000 0000 0000 0000 0000 000	(0001101 ...)



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

Machine precision

The smallest number that, added to 1 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

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

- Truncation

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

Mainly **ROUND OFF**,
due to the finite representation of numbers
in a computer

See also: <https://floating-point-gui.de/>

An example of roundoff+truncation

Numerical derivatives

Calculate the derivative of:

$$f(x) = \sin(x) \text{ in } x = 1$$

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

We can use several algorithms:

$$f'(x) \sim \frac{f_1 - f_{-1}}{2h} \quad (=f'_{sim})$$

$$f'(x) \sim \frac{f_1 - f_0}{h} \quad (=f'_{ds})$$

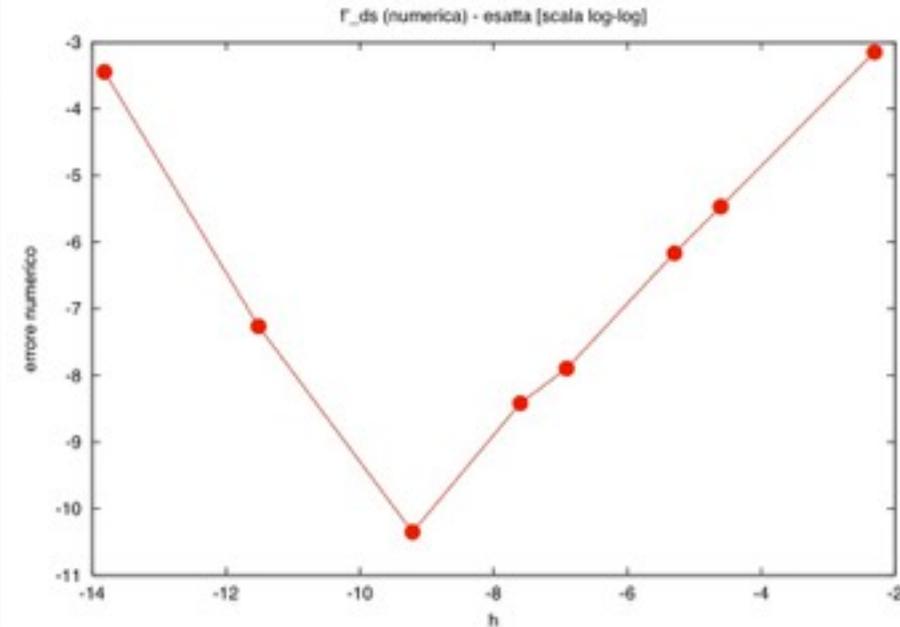
$$f'(x) \sim \frac{f_0 - f_{-1}}{h} \quad (=f'_{sin})$$

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 ($\infty - \infty$)
(a “bad” example: calculate $\exp(-x)$ for $x > 1$ with the standard series with alternate sign)

expressions analytically equivalent
can be NOT numerically equivalent!

$$\sum_{n=1}^{2N} (-1)^n \frac{n}{n+1}$$



$$-\sum_{n=1}^N \frac{2n-1}{2n} + \sum_{n=1}^N \frac{2n}{2n+1}$$

BAD!

for large N:
subtraction between
very large numbers ($\infty - \infty$)

<0

>0



$$\sum_{n=1}^N \frac{1}{2n(2n+1)}$$

OK!

How does your computer make a calculation?

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

In Fortran:

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

since this operation is done within the INTEGERS

$1./2 = ???$ 0.5 !!! **CORRECT**

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

Some programs:

On Moodle:

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
test1-subr-funct.f90 ; test2-subr-funct.f90
test_factorial.f90