



Programmazione Avanzata / 2

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Floating Point Computing



SCAIWhy talking about data formats?



- The "numbers" used in computers are different from the "usual" numbers
- Some differences have known consequences
 - size limits
 - numerical stability
 - algorithm robustness
- Other differences are often misunderstood
 - portability
 - exceptions
 - surprising behaviours with arithmetic







- Computers usually handle bits
- ► An integer number *n* may be stored as a sequence of bits
- Of course, you have a range

$$-2^{r-1} \le n \le 2^{r-1} - 1$$

- Two common sizes
 - ▶ 32 bit: range -2³¹ ≤ n ≤ 2³¹ 1
 - 64 bit: range $-2^{63} \le n \le 2^{63} 1$
- Languages allow for declaring different flavours of integers
 - select the type you need compromizing on avoiding overflow and saving memory
- Is it difficult to have an integer overflow?
 - consider a cartesian discretization mesh (1536 × 1536 × 1536) and a linearized index i

$$0 \le i \le 3623878656 > 2^{31} = 2147483648$$





Bits and Integers / 2



- Fortran "officially" does not let you specify the size of declared data
 - you request kind and the language do it for you
 - in principle very good, but interoperability must be considered with attention
 - and the underlying types are usually just a few of "well known" types
- C standard types do not match exact sizes, too
 - look for int, long int, unsigned int, ...
 - char is an 8 bit integer
 - unsigned integers available, doubling the maximum value $0 \le n \le 2^r 1$





Bits and Reals



- Note: From now on, some examples will consider base 10 numbers just for readability
- Representing reals using bits is not natural
- Fixed size approach
 - select a fixed point corresponding to comma
 - e.g., with 8 digits and 5 decimal places 36126234 gets interpreted as 361.26234
- ► Cons:
 - ▶ limited range: from 0.00001 to 999.99999, spanning 10⁸
 - only numbers having at most 5 decimal places can be exactly represented
- Pros:
 - constant resolution, i.e. the distance from one point to the closest one (0.00001)





Floating point approach



Consider scientific notation

 $n=(-1)^s\cdot m\cdot\beta^e$

$$0.0046367 = (-1)^0 \cdot 4.6367 \cdot 10^{-3}$$

- Represent it using bits
 - one digit for sign s
 - "p-1" digits for significand (mantissa) m
 - "w" digits for exponent e







- Exponent
 - unsigned biased exponent
 - $e_{min} \leq e \leq e_{max}$
 - e_{min} must be equal to $(1 e_{max})$
- Mantissa
 - precision *p*, the digits x_i are $0 \le x_i < \beta$

$$m = \sum_{i=0}^{p-1} x_i \cdot \beta^{-i}$$

"hidden bit" format used for normal values: 1.xx...x

IEEE Name	Format	Storage Size	W	р	e _{min}	e _{max}
Binary32	Single	32	8	24	-126	+127
Binary64	Double	64	11	53	-1022	+1023
Binary128	Quad	128	15	113	-16382	+16383





- Cons:
 - only "some" real numbers are floating point numbers (see later)
- Pros:
 - constant relative resolution (relative precision), each number is represented with the same *relative error* which is the distance from one point to the closest one divided by the number (see later)
 - ► wide range: "normal" positive numbers from 10^{emin} to 9,999..9 · 10^{emax}
- The representation is unique assuming the mantissa is

$$1 \le m < \beta$$

i.e. using "normal" floating-point numbers





Resolution



- The distance among "normal" numbers is not constant
- E.g., $\beta = 2$, p = 3, $e_{min} = -1$ and $e_{max} = 2$:
 - 16 positive "normalized" floating-point numbers





Relative Resolution



- What does it mean "constant relative resolution"?
- Given a number $N = m \cdot \beta^e$ the nearest number has distance

$$R = \beta^{-(p-1)}\beta^e$$

- ▶ E.g., given $3.536 \cdot 10^{-6}$, the nearest (larger) number is $3.537 \cdot 10^{-6}$ having distance $0.001 \cdot 10^{-6}$
- The relative resolution is (nearly) constant (considering 1 ≤ m < β)</p>

$$\beta^{-p} < \frac{R}{N} = \frac{\beta^{-(p-1)}}{m} \le \beta^{-(p-1)}$$





Intrinsic Error



- Not any real number can be expressed as a floating point number
 - because you would need a larger exponent
 - or because you would need a larger precision
- The resolution is directly related to the intrinsic error
 - if p = 4, 3.472 may approximate numbers between 3.4715 and 3.4725, its intrinsic error is 0.0005
 - the instrinsic error is (less than) $(\beta/2)\beta^{-p}\beta^{e}$
 - the relative intrinsic error is

$$(1/2)\beta^{-p} < \frac{(\beta/2)\beta^{-p}}{m} \le (\beta/2)\beta^{-p} = \varepsilon$$

► The intrinsic error ε is also called "machine epsilon" or "relative precision"





Measuring error



When performing calculations, floating-point error may propagate and exceed the intrinsic error

real value	=	3.14145
correctly rounded value	=	3.14
current value	=	3.17

- The most natural way to measure rounding error is in "ulps", i.e. units in the last place
 - e.g., the error is 3 ulps
- Another interesting possibility is using "machine epsilon", which is the relative error corresponding to 0.5 ulps

```
error = 3.17-3.14145 = 0.02855
machine epsilon = 10/2*0.001 = 0.005
relative error = 5.71 \epsilon
```





Handling errors



- Featuring a constant relative precision is very useful when dealing with rescaled equations
- Beware:
 - 0.1 has just one decimal digit using radix 10, but is periodic using radix 2
- the exact binary representation would have a "1100" sequence continuing endlessly:

e = -4; *s* = 110011001100110011001100110011...

When rounded to 24 bits this becomes

e = -4; s = 11001100110011001101, which is actually

0.10000001490116119384765625 in decimal.

- periodicity arises when the fractional part has prime factors not belonging to the radix
- by the way, in Fortran if a is double precision, a=0.2 is badly approximated (use a=0.2d0 instead)
- Beware overflow!
 - you think it will not happen with your code but it may happen
 - exponent range is symmetric: if possibile, perform calculations around 1 is a good idea



Types features



IEEE Name	min	max	ε	С	Fortran
Binary32	1.2E-38	3.4E38	5.96E-8	float	real
Binary64	2.2E-308	1.8E308	1.11E-16	double	real(kind(1.d0))
Binary128	3.4E-4932	1.2E4932	9.63E-35	long double	real(kind=)

- ► There are also "double extended" type and parametrized types
- Extended and quadruple precision devised to limit the round-off during the double calculation of trascendental functions and increase overflow
- Extended and quad support depends on architecture and compiler: often emulated and, hence, slow!
- Decimal with 32, 64 and 128 bits are defined by standards, too
- FPU are usually "conformant" but not "compliant"
- To be safe when converting binary to text specify 9 decimals for single precision and 17 decimal for double



Error propagation



- ► Assume p = 3 and you have to compute the difference 1.01 · 10¹ - 9.93 · 10⁰
- To perform the subtraction, usually a shift of the smallest number is performed to have the same exponent
- First idea: compute the difference exactly and then round it to the nearest floating-point number

 $x = 1.01 \cdot 10^1$; $y = 0.993 \cdot 10^1$

$$x - y = 0.017 \cdot 10^1 = 1.70 \cdot 10^{-2}$$

Second idea: compute the difference with p digits

$$x = 1.01 \cdot 10^1$$
 ; $y = 0.99 \cdot 10^1$

$$x - y = 0.02 \cdot 10^1 = 2.00 \cdot 10^{-2}$$

the error is 30 ulps!





Guard digit



A possibile solution: use the guard digit (p+1 digits)

 $x = 1.010 \cdot 10^{1}$ $y = 0.993 \cdot 10^{1}$ $x - y = 0.017 \cdot 10^{1} = 1.70 \cdot 10^{-2}$

Theorem: if x and y are floating-point numbers in a format with parameters β and p, and if subtraction is done with p + 1 digits (i.e. one guard digit), then the relative rounding error in the result is less than 2 ε.





Cancellation



- When subtracting nearby quantities, the most significant digits in the operands match and cancel each other
- ► There are two kinds of cancellation: catastrophic and benign
 - benign cancellation occurs when subtracting exactly known quantities: according to the previous theorem, if the guard digit is used, a very small error results
 - catastrophic cancellation occurs when the operands are subject to rounding errors
- For example, consider b = 3.34, a = 1.22, and c = 2.28.
 - the exact value of $b^2 4ac$ is 0.0292
 - ▶ but b² rounds to 11.2 and 4ac rounds to 11.1, hence the final answer is 0.1 which is an error by 70ulps
 - the subtraction did not introduce any error, but rather exposed the error introduced in the earlier multiplications.





Cancellation / 2



The expression x² - y² is more accurate when rewritten as (x - y)(x + y) because a catastrophic cancellation is replaced with a benign one

- replacing a catastrophic cancellation by a benign one may be not worthwhile if the expense is large, because the input is often an approximation
- Eliminating a cancellation entirely may be worthwhile even if the data are not exact
- Consider second-degree equations

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

- if $b^2 >> ac$ then $b^2 4ac$ does not involve a cancellation
- ▶ but, if b > 0 the addition in the formula will have a catastrophic cancellation.
- ► to avoid this, multiply the numerator and denominator of x_1 by $-b \sqrt{b^2 4ac}$ to obtain $x_1 = (2c)/(-b \sqrt{b^2 4ac})$ where cineca no catastrophic cancellation occurs

SCA Rounding and IEEE standards



- ► The IEEE standards requires correct rounding for:
 - addition, subtraction, mutiplication, division, remainder, square root
 - conversions to/from integer
- ► The IEEE standards recommends correct rounding for:

► e^x , $e^x - 1$, 2^x , $2^x - 1$, $\log_{\alpha}(\phi)$, $1/\sqrt{(x)}$, sin(x), cos(x), tan(x),....

Remember: "No general way exists to predict how many extra digits will have to be carried to compute a transcendental expression and round it correctly to some preassigned number of digits" (W. Kahan)



Special values



- Zero: signed
- Infinity: signed
 - overflow, divide by 0
 - ► Inf-Inf, Inf/Inf, $0 \cdot Inf \rightarrow NaN$ (indeterminate)
 - Inf op a → Inf if a is finite
 - a / Inf \rightarrow 0 if a is finite
- NaN: not a number!
 - Quiet NaN or Signaling NaN
 - ▶ e.g. √a with a < 0</p>
 - ► NaN op a → NaN or exception
 - NaNs do not have a sign: they aren't a number
 - The sign bit is ignored
 - NanS can "carry" information





Zero and Denormals



- ► Considering positve numbers, the smallest "normal" floating point number is n_{smallest} = 1.0 · β^{e_{min}}
- In the previous example it is 1/2



- At least we need to add the zero value
 - there are two zeros: +0 and -0
- When a computation result is less than the minimum value, it could be rounded to zero or to the minimum value





Zero and Denormals / 2



- Another possibility is to use denormal (also called subnormal) numbers
 - ► decreasing mantissa below 1 allows to decrease the floating point number, e.g. 0.99 · β^emin, 0.98 · β^emin, ..., 0.01 · β^emin
 - subnormals are linearly spaced and allow for the so called "gradual underflow"
- Pro: k/(a − b) may be safe (depending on k) even is a − b < 1.0 · β^{e_{min}}
- Con: performance of denormals are significantly reduced (dramatic if handled only by software)
- Some compilers allow for disabling denormals
 - Intel compiler has -ftz: denormal results are flushed to zero
 - automatically activated when using any level of optimization!





Walking Through



Double precision: w=11 ; p=53

0x000000000000000000	+zero
0x000000000000000000000000000000000000	smallest subnormal
0x000ffffffffff	largest subnormal
0x001000000000000	smallest normal
0x001fffffffffff	
0x0020000000000000	2 X smallest normal
0x7feffffffffff	largest normal
0x7ff00000000000000	+infinity





Walking Through



0x7ff000000000000	NaN
0x7fffffffffff	NaN
0x8000000000000000	-zero
0x800000000000000	negative subnormal
0x800ffffffffff	'largest' negative subnormal
0x801000000000000	'smallest' negative normal
0xfff0000000000000000	-infinity
0xfff000000000001	NaN
0xffffffffffff	NaN





Error-Free Transformations



- An error-free transformation (EFT) is an algorithm which determines the rounding error associated with a floating-point operation
- E.g., addition/subtraction

 $a + b = (a \oplus b) + t$

where \oplus is a symbol for floating-point addition

- Under most conditions, the rounding error is itself a floating-point number
- An EFT can be implemented using only floating-point computations in the working precision





EFT for Addition



FastTwoSum: compute a + b = s + t where

|**a**| ≥ |**b**|

 $s = a \oplus b$







EFT for Addition / 2



- ▶ No requirements on |a| or |b|
- Beware: avoid compiler unsafe optimizations!





Summation techniques



Condition number

$$C_{sum} = rac{\sum |a_i|}{|\sum a_i|}$$

- If C_{sum} is "not too large", the problem is not ill conditioned and traditional methods may suffice
- But if it is "too large", we want results appropriate to higher precision without actually using a higher precision
- But if higher precision is available, consider to use it!
 - beware: quadruple precision is nowadays only emulated





Traditional summation



$$s = \sum_{i=0}^{n} x_i$$

```
double Sum( const double* x, const int n ) {
    int i;
    for ( i = 0; i < n; i++ ) {
        Sum += x[ i ];
    }
    return Sum;
}</pre>
```

- Traditional Summation: what can go wrong?
 - catastrophic cancellation
 - magnitude of operands nearly equal but signs differ
 - loss of significance
 - small terms encountered when running sum is large
 - the smaller terms don't affect the result
 - but later large magnitude terms may reduce the running sum





Sorting and Insertion



- Reorder the operands; sort by
 - Increasing magnitude value
- Insertion
 - First sort by magnitude
 - Remove the first two item and compute their sum
 - Insert the result on the list, keeping list sorted
 - Repeat until only one element is left on the list
- Many variations





Kahan summation



- Based on FastTwoSum and TwoSum techniques
- Knowledge of the exact rounding error in a floating-point addition is used to correct the summation
- Compensated Summation









- Many variations known (Knutht, Priest,...)
- Sort the values and sum starting from smallest values (for positive numbers)
- Other techniques (distillation)
- Use a greater precision or emulate it (long accumulators)
- Similar problems for Dot Product, Polynomial evaluation,...







- Underflow
 - Absolute value of a non zero result is less than the minimum value (i.e., it is subnormal or zero)
- Overflow
 - Magnitude of a result greater than the largest finite value
 - ► Result is ±∞
- Division by zero
 - a/b where a is finite and non zero and b=0
- Inexact
 - Result, after rounding, is not exact
- Invalid
 - an operand is sNaN, square root of negative number or combination of infinity







- Let us say you may produce a NaN
- What do you want to do in this case?
- First scenario: go on, there is no error and my algorithm is robust
- E.g., the function maxfunc compute the maximum value of a scalar function f(x) testing each function value corresponding to the grid points g(i)

call maxfunc(f,g)

- to be safe I should pass the domain of f but it could be difficult to do
- I may prefer to check each grid point g(i)
- if the function is not defined somewhere, I will get a NaN (or other exception) but I do not care: the maximum value will be correct





Handling exceptions / 2



- Second scenario: ops, something went wrong during the computation...
- (Bad) solution: complete your run and check the results and, if you see NaN, throw it away
- (First) solution: trap exceptions using compiler options (usually systems ignore exception as default)
- Some compilers allow to enable or disable floating point exceptions
 - Intel compiler: -fpe0: Floating-point invalid, divide-by-zero, and overflow exceptions are enabled. If any such exceptions occur, execution is aborted.
 - GNU compiler:

-ffpe-trap=zero, overflow, invalid, underflow

- very useful, but the performance loss may be material!
- use only in debugging, not in production stage





Handling exceptions / 3



- (Second) solution: check selectively
 - ► each *N*_{check} time-steps
 - the most dangerous code sections
- Using language features to check exceptions or directly special values (NaNs,...)
 - the old print!
 - Fortran (2003): from module ieee_arithmetic, ieee_is_nan(x), ieee_is_finite(x)
 - C: from <math.h>, isnan or isfinite, from C99 look for fenv.h
 - do not use old style checks (compiler may remove them):

```
int IsFiniteNumber(double x) {
    return (x <= DBL_MAX && x >= -DBL_MAX);
}
```







Floating-point control



- Why doesn't my application always give the same answer?
 - inherent floating-point uncertainty
 - we may need reproducibility (porting, optimizing,...)
 - accuracy, reproducibility and performance usually conflict!
- Compiler safe mode: transformations that could affect the result are prohibited, e.g.
 - x/x = 1.0, false if $x = 0.0, \infty, NaN$
 - x y = -(y x) false if x = y, zero is signed!
 - ► *x* − *x* = 0.0 ...
 - ► *x* * 0.0 = 0.0 ...



Floating-point control / 2



- An important case: reassociation is not safe with floating-point numbers
 - (x + y) + z = x + (y + z): reassociation is not safe
 - compare

-1.0+1.0e-13+1.0 = 1.0-1.0+1.0e-13 = 1.0e-13+1.0-1.0

- a * b/c may give overflow while a * (b/c) does not
- Best practice:
 - select the best expression form
 - promote operands to the higher precision (operands, not results)



Floating-point control / 3



- Compilers allow to choose the safety of floating point semantics
- GNU options (high-level):

-f[no-]fast-math

- It is off by default (different from icc)
- Also sets abrupt/gradual underflow (FTZ)
- Components control similar features, e.g. value safety

(-funsafe-math-optimizations)

For more detail

http://gcc.gnu.org/wiki/FloatingPointMath





Floating-point control / 4



- Intel options:
 - -fp-model <type>
 - fast=1: allows value-unsafe optimizations (default)
 - fast=2: allows additional approximations
 - precise: value-safe optimizations only
 - strict: precise + except + disable fma
- Also pragmas in C99 standard

#pragma STDC FENV_ACCESS etc





Endianness



Which is the ordering of bytes in memory? E.g.,

-1267006353 ===> 1011010001111011000010001101111

- ► Big endian: 10110100 01111011 00000100 01101111
- Little endian: 01101111 00000100 01111011 10110100
- Other exotic layouts (VAX,...) nowadays unusual
- Limits portability
- Possibile solutions
 - conversion binary to text and text to binary
 - compiler extensions(Fortran):
 - HP Alpha, Intel: -convert big_endian | little_endian
 - PGI: -byteswapio
 - Intel, NEC: F_UFMTENDIAN (variabile di ambiente)
 - explicit reoredering
 - conversion libraries



SCAI C and Fortran data portability



- ► For C Standard Library a file is written as a stream of byte
- In Fortran file is a sequence of records:
 - each read/write refer to a record
 - there is record marker before and after a record (32 or 64 bit depending on file system)
 - remember also the different array layout from C and Fortran
- Possible portability solutions:
 - read Fortran records from C
 - perform the whole I/O in the same language (usually C)
 - use Fortran 2003 access='stream'
 - use I/O libraries







- Single, Double or Quad?
 - maybe single is too much!
 - computations get (much) slower when increasing precision, storage increases and power supply too
- Famous story
 - Patriot missile incident (2/25/91) . Failed to stop a scud missile from hitting a barracks, killing 28
 - System counted time in 1/10 sec increments which doesn't have an exact binary representation. Over time, error accumulates.
 - The incident occurred after 100 hours of operation at which point the accumulated errors in time variable resulted in a 600+ meter tracking error.
- Wider floating point formats turn compute bound problems into memory bound problems!



Which precision do I need?/2



- Programmers should conduct mathematically rigorous analysis of their floating point intensive applications to validate their correctness
- Training of modern programmers often ignores numerical analysis
- Useful tricks
 - Repeat the computation with arithmetic of increasing precision, increasing it until a desired number of digits in the results agree
 - Repeat the computation in arithmetic of the same precision but rounded differently, say Down then Up and perhaps Towards Zero, then compare results
 - Repeat computation a few times in arithmetic of the same precision but with slightly different input data, and see how widely results vary







- A "correct" approach
- Interval number: possible values within a closed set

 $\mathbf{X} \equiv [\mathbf{X}_L, \mathbf{X}_R] := \{ \mathbf{X} \in \mathbb{R} | \mathbf{X}_L \le \mathbf{X} \le \mathbf{X}_R \}$

- ▶ e.g., 1/3=0.33333 ; 1/3 ∈ [0.3333,0.3334]
- Operations: let x = [a, b] and y = [c, d]
 - Addition x + y = [a, b] + [c, d] = [a + c, b + d]
 - Subtraction x y = [a, b] [c, d] = [a -d, b -c]
 - ▶ ...
- Properties are interesting and can be applied to equations
- Interval Arithmetic has been tried for decades, but often produces bounds too loose to be useful
- A possible future
 - chips supporting variable precision and uncertainty tracking
 - runs software at low precision, tracks accuracy and reruns computations automatically if the error grows too large.





References



- N.J. Higham, Accuracy and Stability of Numerical Algorithms 2nd ed., SIAM, capitoli 1 e 2
- D. Goldberg, What Every Computer Scientist Should Know About Floating-Point Arithmetic, ACM C.S., vol. 23, 1, March 1991 http://docs.oracle.com/cd/E19957-01/806-3568/ncg_goldberg.html
- ► W. Kahan http://www.cs.berkeley.edu/ wkahan/
- Standards: http://grouper.ieee.org/groups/754/







The code in summation.cpp/f90 initializes an array with an ill-conditioned sequence of the order of

100,-0.001,-100,0.001,....

- Simple and higher precision summation functions are implemented
- Implement Kahan algorithm in C++ or Fortran
- Compare the accuracy of the results





Hands-on: C++ Solution



```
REAL TYPE summation kahan ( const REAL TYPE a[],
                        const size_t n_values )
 REAL TYPE s = a[0];
                              // sum
 REAL TYPE t = 0;
                              // correction term
 for( int i = 1; i < n values; i++ ) {
     REAL_TYPE y = a[ i ] - t; // next term "plus" correction
     REAL_TYPE z = s + y;
                             // add to accumulated sum
     t = (z - s) - y;
                              // t <- -(low part of y)
                              // update sum
     s = z;
 return s;
```

Summation simple : 35404.9609375000000000

Summation Kahan : 35402.8515625000000000 Summation higher : 35402.8554687500000000



SCA Hands-on: Fortran Solution

uperComputing Applications and Innovation



```
function sum_kahan(a,n)
    integer :: n
    real(my_kind) :: a(n)
    real(my_kind) :: s,t,y,z
    s=a(1)
                       ! sum
   t=0._my_kind
                      ! correction term
   do i=2,n
      y = a(i) - t ! next term "plus" correction
      z = s + y ! add to accumulated sum
      t = (z-s) - y ! t < - -(low part of y)
                      ! update sum
      s = z
   enddo
    sum kahan = s
end function sum kahan
```

Summation simple: -13951.87109375000000 Summation Kahan: -13951.91113281250000 Summation Higher: -13951.91210937500000





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