Computing with Floating Point

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15/04/2016.99999

Introduction
Common misconceptions
Floating-point as it should be: the IEEE-754 standard
Floating-point as it is:
   processors,
   languages and compilers
Conclusion and perspective
To probe further:

- Goldberg: *What Every Computer Scientist Should Know About Floating-Point Arithmetic*  
  (Google will find you several copies)
- The web page of William Kahan at Berkeley.
- The web page of the AriC group.

Handbook of Floating-Point Arithmetic, by Muller et al.
Introduction

Common misconceptions

Floating-point as it should be: the IEEE-754 standard

Floating-point as it is:

processors,

languages and compilers

Conclusion and perspective
From $9.10938215 \times 10^{-31}$ kg to $6.0221415 \times 10^{23}$ mol$^{-1}$

- Multiplication algorithm is trivial
  - (but typically involves some rounding)
- Addition algorithm is slightly more complex
  - align the two numbers to the same exponent
  - perform the addition/subtraction
  - optionally, round

Golden rules (according to my physics teachers)

- The number of digits we write is the number of digits we trust
- Each number has a unit attached to it
Scientific notation

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Floating-point in your computer is just that

... with two main differences:

**Binary instead of decimal**

Since the Zuse Z1 (1938)

1.1111110000110000110000011000 \times 2^{78}
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**Binary instead of decimal**

Since the Zuse Z1 (1938)

\[1.11111110000110000110000011000 \times 2^{78}\]

The computer doesn’t manage the golden rules

- No unit attached (Mars Climate Orbiter crash in 1999)
- The numbers of bits we manipulate is the number of bits we have (correct or wrong)
A floating-point number is a rational:

\[ x = (-1)^s \times m \times \beta^e \]

- **\( \beta \)** is the radix
  - 10 in your calculator, your bank’s computer, and (usually) your head
  - 2 in most computers (binary arithmetic)
- **\( s \in \{0, 1\} \)** is a sign bit
- **\( m \)** is the *mantissa*, a fixed-point number of \( p \) digits in radix \( \beta \):
  \[ m = d_0, d_1d_2...d_{p-1} \]
- **\( e \)** is the exponent, a signed integer between \( e_{\text{min}} \) and \( e_{\text{max}} \)
  - ... how it is represented is mostly irrelevant
Let’s be formal

A floating-point number is a rational:

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\( p \) specifies the precision of the format,
\[ [e_{\text{min}}...e_{\text{max}}] \text{ specifies its dynamic.} \]
An infinity of equivalent representations:

- \( 6.0221415 \times 10^{23} \)
- \( 60221415 \times 10^{16} \)
- \( 602214150000000000000000 \times 10^0 \)
- \( 0.00000060221415 \times 10^{30} \)

Imposing a unique representation will simplify comparisons.

Which one is best?

- Leading and trailing zeroes are useless (to the computation)
- The first representation is preferred
  - one and only one non-zero digit before the point
  - then the exponent gives the order of magnitude

In radix 2, if the first digit is not a zero, it is a one

no need to store it.
Mainstream formats of the IEEE-754 standard

<table>
<thead>
<tr>
<th>Name</th>
<th>binary32</th>
<th>binary64</th>
</tr>
</thead>
<tbody>
<tr>
<td>old name</td>
<td>single precision</td>
<td>double precision</td>
</tr>
<tr>
<td>C/C++ name</td>
<td>float</td>
<td>double</td>
</tr>
<tr>
<td>total size</td>
<td>32 bits</td>
<td>64 bits</td>
</tr>
<tr>
<td>$p$</td>
<td>24</td>
<td>53</td>
</tr>
<tr>
<td>$2^{-p}$</td>
<td>$\approx 6 \cdot 10^{-8}$</td>
<td>$\approx 10^{-16}$</td>
</tr>
<tr>
<td>$w_E$</td>
<td>8</td>
<td>11</td>
</tr>
<tr>
<td>$e_{\min}, e_{\max}$</td>
<td>$-126, +127$</td>
<td>$-1022, +1023$</td>
</tr>
<tr>
<td>smallest</td>
<td>$\approx 1.401 \times 10^{-45}$</td>
<td>$\approx 4.941 \times 10^{-324}$</td>
</tr>
<tr>
<td>largest</td>
<td>$\approx 3.403 \times 10^{38}$</td>
<td>$\approx 1.798 \times 10^{308}$</td>
</tr>
</tbody>
</table>

MSB

<table>
<thead>
<tr>
<th>S</th>
<th>E</th>
<th>F</th>
</tr>
</thead>
</table>

1 bit $w_E$ bits $p - 1$ bits

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Computing with Floating Point
Non mainstream formats in IEEE754-2008

- binary16 (an *exchange* format, don't compute with it)
- binary128 (currently unsupported by hardware)
- possibly extended formats
- decimal formats
  - decimal32, decimal64
The decimal fiasco

Much debated in the early 2000 as the IEEE-754 standard was revised

- intended to support financial calculations
  (interest rates are given in decimal)
- supported in software on intel, in hardware in some IBM mainframes
  - first mess: two different encodings
- ... but money is fixed-point, not floating-point
  - second mess: non-unicity of representation
- My advice:
  - stay clear of decimal numbers,
  - and count your money in a 64-bit integer, it should fit.
Floating point is something well defined and well understood

- The set of floating-point numbers is well defined for 32- or 64-bit formats.

- The operations are well-defined as well.
  - For any real $x$, we may define a function $\circ(x)$ that returns the FP number that is the nearest to $x$.
  - Then, FP addition of $a$ and $b$ is defined as $\circ(a + b)$.
  - ... in other words: as good as possible.
  - (same for $+,-,\times,/,$ $\sqrt{\cdot}$)

- All this in a standard (IEEE-754) supported by virtually all computing systems.

*We can build serious math and serious proofs on top of this.*
• sometimes \texttt{real}, \texttt{real*8},
• sometimes \texttt{float},
- sometimes `real`, `real*8`,
- sometimes `float`,
- sometimes silly names like `double` or even `long double`
The numeric types in C:
- **char** (the 8-bit integer) is an abbreviated noun (character) from typography
  - unsigned char ?
- you can add two char
- **int** is an abbreviated noun (integer) from mathematics
  - although 2147483647 +1 = -2147483648
- short and long are adjectives
- **float** is a verb, at least it is a computer term
- double means double what?
- long double is not even syntactically correct in english
Parenthesis: good language design

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After so much nonsense, if you’re lost, it is not your fault
- `float`=binary32, `double`=binary64
- Also, in doubt, use `int` types from `<stdint.h>`, such as `uint32_t`. 
Common misconceptions

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À tout seigneur, tout honneur

From Kahan’s lecture notes (on the web):

1. What you see is often not what you have.
2. What you have is sometimes not what you wanted.
3. If what you have hurt you, you will probably never know how or why.
4. Things go wrong too rarely to be properly appreciated, but not rarely enough to be ignored.
Floating-point numbers are real numbers

- Of course they are, since they are rationals.
- However, many properties on the reals are no longer true on the floating-point numbers.

To start with: Floating-point addition is not associative.

A perfectly sensible floating-point program (Malcolm-Gentleman)

```plaintext
A := 1.0;
B := 1.0;
while ((A+1.0)-A)-1.0 = 0.0
    A := 2 * A;
while ((A+B)-A)-B <> 0.0
    B := B + 1.0;
return(B)
```
To reason about this kind of programs,

- draw an $x$ axis with the exponents
- position the significands as rectangles of fixed size along this axis
- reason about the position of the result mantissa
- draw the exact results, and the rounded results

**Exercise**

Illustrate that floating-point addition is not associative
Common misconception 0.5

All rational numbers can be represented as floating-point numbers 1/3 cannot. Worst, 1/10, 1/100 etc cannot either. Remember that FP numbers are binary. Many bugs in Excel are due to its attempts to hide this fact.

Exercise

What is the error of representing $\pi$ as a binary32 number?
- define “error”
- compute a tight bound.
The Patriot bug

In 1991, a Patriot failed to intercept a Scud (28 killed).

- The code worked with time increments of 0.1 s.
- But 0.1 is not representable in binary.
- In the 24-bit format used, the number stored was 0.099999904632568359375
- The error was 0.0000000953.
- After 100 hours = 360,000 seconds, time is wrong by 0.34s.
- In 0.34s, a Scud moves 500m

(similar problems have been discovered in civilian air traffic control systems, after near-miss incidents)

Test: which of the following increments should you use?

<table>
<thead>
<tr>
<th>10</th>
<th>5</th>
<th>3</th>
<th>1</th>
<th>0.5</th>
<th>0.25</th>
<th>0.2</th>
<th>0.125</th>
<th>0.1</th>
</tr>
</thead>
</table>
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Floating-point programs may be deterministic and portable... but not without work.
An FP program that behaves deterministically probably returns the correct result.
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... probably...
An FP program that behaves deterministically probably returns the correct result.

... probably...

Two illustrations:

- Muller’s recurrence:

  \[ f(y, z) = 108 - (815 - 1500/z)/y \]

  \[ x_0 = 4 \]

  \[ x_1 = 4.25 \]

  \[ x_i = f(x_{i-1}, x_{i-2}) \]

- Vancouver Stock Exchange FP Fail
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- This is much easier if an FP number only represents itself, and if each operation is as accurate as possible.
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If you are able to define accurately the “real value” corresponding to every single variable in your 100,000 lines of code, you definitely know more than the computer.
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- Many are exact, we know who they are, and we may even force them into our programs
- A consequence of IEEE-754 operation specification:
  If the exact result of an operation is representable as a floating-point number, then the operation will return this exact result.
Examples of exact operations

Decimal, 4 digits of mantissa

- $4.200 \cdot 10^1 \times 1.000 \cdot 10^1 = 4.200 \cdot 10^2$
- $4.200 \cdot 10^1 \times 1.700 \cdot 10^6 = 7.140 \cdot 10^7$
- $1.234 + 5.678 = 6.912$
- $1.234 - 1.233 = 0.001 = 1.000 \cdot 10^{-3}$
My first cancellation

\[ 1.234 - 1.233 = 0.001 = 1.000 \cdot 10^{-3} \]

- On one hand, this operation is exact
  - if I consider that a floating-point number represents only itself
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- On the other hand, the 0s in the mantissa of the result are probably meaningless
  - if I consider that, in the “real world”, my two input numbers would have had digits beyond these 4.

So, is this situation good or bad?
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So, is this situation good or bad?

Usually good, but bad if the following computation depends on these meaningless digits
Write a program that solves the quadratic equation

Formulas I learnt in school:

\[ \delta = b^2 - 4ac \]

if \( \delta \geq 0 \), \( r = \frac{-b \pm \sqrt{\delta}}{2a} \)

- There are two subtractions here. Can one of them lead to problematic cancellation? In which cases?
- If yes, try and change the formula.
Misconception 4:
16 digits should be enough for anybody

Double precision (binary64) provides roughly 16 decimal digits.

Count the digits in the following

- Definition of the second: *the duration of* 9,192,631,770 *periods of the radiation corresponding to the transition between the two hyperfine levels of the ground state of the cesium 133 atom.*

- Definition of the metre: *the distance travelled by light in vacuum in* 1/299,792,458 *of a second.*

- Most accurate measurement ever (another atomic frequency) to 14 decimal places

- Most accurate measurement of the Planck constant to date: to 7 decimal places
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- Most accurate measurement ever (another atomic frequency) to 14 decimal places
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- The gravitation constant $G$ is known to 3 decimal places only
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Yet another variant: $\pi = 3.1416$ at the beginning of your program

- Sometimes it’s enough
- Consider $\sin(2\pi Ft)$ as time passes...
- The standard sine implementation needs to store 1440 bits (420 decimal digits) of $1/\pi$...
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(I’ll have one slide on decimal/binary conversion, don’t worry)
Vendors would sell us hardware that we don’t need?

- This PC computes $10^9$ operations per second (1 gigaflops)
- This is a lot. Kulisch:
  - print the numbers in 100 lines of 5 columns double-sided: 1000 numbers/sheet
  - 1000 sheets ≈ a heap of 10 cm
  - $10^9$ flops ≈ heap height speed of 100m/s, or 360km/h
  - A teraflops ($10^{12}$ op/s) machine builds in one second a pile of paper to the moon.
  - Current top 500 computers reach the petaflop ($10^{16}$ op/s)

- Relationship to precision?
Where does precision go?

- each operation may involve an error of the weight of the last digit (relative error of $10^{-16}$)
- If you are computing a big sum, these errors add up.
- In a Gflops machine, after one second you have lost 9 digits of your result (remains 6).
- In a petaflops machine, you may have lost all your digits in 0.1s.

Managing this is a big challenge of current HPC
Estimated diameter of the Universe
\[ \frac{\text{Planck length}}{\approx 10^{62}} ; \]

A double-precision FP number holds numbers up to \(10^{308}\);
No need to worry about over/underflow
Common misconception 5

Estimated diameter of the Universe
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⊕ Over/underflows do happen in real code:
  - geometry (very flat triangles, etc)
  - statistics/probabilities
  - intermediate values, approximation formulae
  - ...
Common misconception 5

\[
\frac{\text{Estimated diameter of the Universe}}{\text{Planck length}} \approx 10^{62} = \ldots
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Exercise

You need to compute

\[
\frac{x^2}{\sqrt{x^3 + 1}}
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What happens for large values of \( x \) ?
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  - \( \sqrt{+\infty} = +\infty \)
  - \( \frac{\text{finite}}{+\infty} = 0 \)
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  - \( \sqrt{+\infty} = +\infty \)
  - \( \frac{\text{finite}}{+\infty} = 0 \)

- Here again, the solution is
  - to expect the problem before it hurts you
  - and to protect the computation with a test which returns \( \sqrt{x} \)
    for large values
  - (a more accurate result, obtained faster...)

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Computing with Floating Point
Common misconceptions 6

My good program gives wrong results, it’s because of approximate floating-point arithmetic.

- Mars Climate Orbiter crash
- Naive two-body simulation
Arithmetic is not always the culprit

- Ask first-year students to write a simulation of one planet around a sun

\[
\begin{align*}
x(t) & := v(t) \delta t \\
v(t) & := a(t) \delta t \\
a(t) & := \frac{K}{||x(t)||^2}
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- You always get rotating ellipses
- Analysing the simulation shows that it creates energy.
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The dark ages of anarchy

In the ancient times (before 1985), there were as many implementations of floating-point as there were machines

- no hope of portability
- little hope of proving results e.g. on the numerical stability of a program
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- horror stories: \( \arcsin \left( \frac{x}{\sqrt{x^2 + y^2}} \right) \) could segfault on a Cray
- therefore, little trust in FP-heavy programs
Rationale behind the IEEE-754-85 standard

- Enable data exchange
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- Ensure portability
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  - People will assume that $x + 0 == x$
  - People will assume that $x == y \iff x - y == 0$
  - People will assume that $\frac{x}{\sqrt{x^2+y^2}} \leq 1$
  - ...

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Obviously, need to specify not only the number formats but also the operations on these numbers.
Desirable properties:

- an FP number has a unique representation
- every FP number has an opposite
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Normal numbers

\[ x = (-1)^s \times 2^e \times 1.m \]

For unicity of representation, we impose \( d_0 \neq 0 \).
(In binary, \( d_0 \neq 0 \iff d_0 = 1 \): It needn’t be stored.)
Desirable properties:
- representation of 0
- representations of $\pm \infty$ (and therefore $\pm 0$)
- standardized behaviour in case of overflow or underflow.
  - return $\infty$ or 0, and raise some flag/exception
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- representation of 0
- representations of $\pm\infty$ (and therefore $\pm0$)
- standardized behaviour in case of overflow or underflow.
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- representations of $NaN$: Not a Number
  (result of $0^0$, $\sqrt{-1}$, ...)
  - Quiet NaN
  - Signalling NaN
Choice of binary representation

Desirable property: the order of FP numbers is the lexicographical order of their binary representation

Binary encoding of positive numbers

- place exponent at the MSB (left of significand)
- infinity is larger than any normal number: code it with the largest exponent $111...1_2$
- zero is smaller than any normal number: code it with the smallest exponent $000...0_2$
- for normal exponents: biased representation
  - assume $w_E$ bits of exponent
  - exponent field $E \in \{0...2^{w_E} - 1\}$ codes for exponent $e = E - \text{bias}$
  - In IEEE-754, bias for significand in $[1, 2)$ is $\text{bias} = 2^{w_E-1} - 1 = 0111...1_2$
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How to code NaNs? Significand of infinity? Significand of 0? ...
Subnormal numbers

\[ x = (-1)^s \times 2^e \times 1.m \]

Desirable properties:

- \( x == y \iff x - y == 0 \)
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Subnormal numbers

If \( E = 00...0_2 \),
- the exponent remains stuck to \( e_{\text{min}} \)
- and the implicit \( d_0 \) is equal to 0:
  \[ x = (-1)^s \times 2^{e_{\text{min}}} \times 0.m \]
3 bits of exponent, 4 bits of fraction (4+1 bits of significand)

<table>
<thead>
<tr>
<th>exp fraction</th>
<th>value</th>
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<td>000 0000</td>
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<td>000 0001</td>
<td>0.0001 \cdot 2^{e_{\min}}</td>
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<tr>
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<tr>
<td>111 0000</td>
<td>+\infty</td>
<td></td>
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NextAfter obtained by adding 1 to the binary representation

from 0 to +\infty
Desirable properties:

- If \(a + b\) is a FP number, then \(a \oplus b\) should return it.
- Rounding should be monotonic.
- Rounding should not introduce any statistical bias.
- Sensible handling of infinities and NaNs.
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An unambiguous choice: this is the best that the format allows.
Operations

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An unambiguous choice: this is the best that the format allows.

Three other rounding modes: to $+\infty$, to $-\infty$, to 0, with similar correct rounding requirement (and no tie problem).
Oh, and by the way
the standard should be implementable

(back in 1985 this was a bit controversial)

- The exact sum of two FP numbers of precision $p$ can be stored on $\approx 2p$ bits only
- Same for the exact product

Most controversial point:
Subnormal handling is indeed complex/expensive, and has long been trapped to software/microcode
Correctly rounded elementary functions were considered not implementable then
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  - to compute $x/y$, first compute $(q, r)$ such that $x = yq + r$
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  - to compute $\sqrt{x}$, first compute $(s, r)$ such that $x = s^2 + r$
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Correctly rounded elementary functions were considered not implementable then
Let $x$ and $y$ be FP numbers.

- Sterbenz Lemma: if $x/2 < y < 2x$ then $x \ominus y = x - y$
Let $x$ and $y$ be FP numbers.

- **Sterbenz Lemma**: if $x/2 < y < 2x$ then $x \ominus y = x - y$

- The rounding error when adding $x$ and $y$:
  
  $r = (x + y) - (x \oplus y)$ is an FP number, and if $x \geq y$ it may be computed as

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- $\sqrt{x \otimes x + y \otimes y} \geq x$
A few theorems (useful or not)

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- ...
Floating-point format in radix $\beta$ with $p$ digits of significand
Suppose $x$ and $y$ are positive.
Notation using integral significands:

$$x = M_x \times \beta^{e_x-p+1},$$

$$y = M_y \times \beta^{e_y-p+1},$$

with

$$\begin{cases} 
eq \leq e_x \leq e_{\text{max}} \\
eq \leq e_y \leq e_{\text{max}} \\
o < M_x < \beta^p - 1 \\
o < M_y < \beta^p - 1. \end{cases}$$
Suppose \( y \leq x \) therefore \( e_y \leq e_x \): define \( \delta = e_x - e_y \)

\[
x - y = \left( M_x \beta^\delta - M_y \right) \times \beta^{e_y-p+1}.
\]

Define \( M = M_x \beta^\delta - M_y \)

- \( x \geq y \) implies \( M \geq 0 \);
- \( x \leq 2y \) implies \( x - y \leq y \), hence \( M \beta^{e_y-p+1} \leq M_y \beta^{e_y-p+1} \);

therefore,

\[
M \leq M_y \leq \beta^p - 1.
\]

So \( x - y \) is equal to \( M \times \beta^{e-p+1} \) with \( e_{\min} \leq e \leq e_{\max} \) and \( |M| \leq \beta^p - 1 \). This shows that \( x - y \) is a floating-point number, which implies that it is exactly computed.
We haven’t used the rounding mode?!?

- We just proved that the mathematical result is representable
- Any rounding mode ⨅ verifies: if \( Z \) is representable, then
  \[ \circ(Z) = Z \]
- Sterbenz lemma is true for any rounding mode.
Remarks on this proof

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- We need subnormals, of course.

(Normal numbers have an integral significand such that $\beta^{p-1} \leq M \leq \beta^p - 1$ and we couldn’t prove the left inequality)
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- We don’t care about the binary encoding (only that there is an $e_{\text{min}}$)
Writing a constant in decimal can be safe enough if you are aware of the following.

- Any binary FP number can be written in decimal (given enough digits)
  - first rewrite $m \cdot 2^e = (5^{-e} m) \cdot 10^e$
  - then find some $k$ such that $10^k \cdot m \cdot 2^e$ is an integer $n$
  - then $m \cdot 2^e = n \cdot 10^{e-k}$

- The reciprocal is not true (e.g. 0.1)

- Modern compilers are well behaved:
  - They will consider all the decimal digits you give them
  - They will round the decimal constant you provide to the nearest FP number
Error-free write-read cycle

Theorem
Writing a binary32 (resp. binary64 number) to file on 10 (resp. 20) decimal digits guarantees that the exact same number will be read back.

(Actually the minimal decimal sizes are 9 and 17 digits)
We have a standard for FP, and it seems well thought out.

(all we have seen was already in the 1985 version – more on the 2008 revision later)
The conclusion so far

- We have a standard for FP, and it seems well thought out.
- (all we have seen was already in the 1985 version – more on the 2008 revision later)

Let us try to use it.
Floating-point as it is

Introduction

Common misconceptions

Floating-point as it should be: the IEEE-754 standard

Floating-point as it is:

processors,

languages and compilers

Conclusion and perspective
Let us compile the following C program:

```c
float ref, index;

ref = 169.0 / 170.0;

for (i = 0; i < 250; i++) {
    index = i;
    if ((index / (index + 1.0)) == ref )
        printf("Success!");

    printf("i=%d\n",i);
}
```

Florent de Dinechin, Florent.de-Dinechin@insa-lyon.fr Computing with Floating Point
Equality test between FP variables is dangerous.

Or,

If you can replace \( a==b \) with \( (a-b)\text{<}\text{epsilon} \) in your code, do it!
Equality test between FP variables is dangerous.
Or,
If you can replace \(a==b\) with \((a-b)<\text{epsilon}\) in your code, do it!

A physical point of view:
*Given two coordinates \((x, y)\) on a snooker table,*
The probability that the ball stops at position \((x, y)\) is always zero.
Equality test between FP variables is dangerous.

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If you can replace \( a==b \) with \((a-b) < \epsilon\) in your code, do it!

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*Given two coordinates \((x, y)\) on a snooker table, the probability that the ball stops at position \((x, y)\) is always zero.*

Still, on this expensive laptop, FP computing is not straightforward, even within such a small program.
First conclusion

Equality test between FP variables is dangerous.
Or,
If you can replace \(a==b\) with \((a-b)<\epsilon\) in your code, do it!

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*Given two coordinates \((x, y)\) on a snooker table, the probability that the ball stops at position \((x, y)\) is always zero.*

Still, on this expensive laptop, FP computing is not straightforward, even within such a small program.

Go fetch me the person in charge
Who is in charge of ensuring the standard?

- The processor
  - has internal FP registers,
  - performs basic FP operations,
  - raises exceptions,
  - writes results to memory.
Who is in charge of ensuring the standard?

- The processor
- The operating system
  - handles exceptions
  - computes functions/operations not handled directly in hardware
    - most elementary functions (sine/cosine, exp, log, ...),
    - sometimes divisions and square roots, and even basic operations
    - sometimes subnormal numbers
  - handles floating-point status: precision, rounding mode, ...
    - older processors: global status register
    - more recent FPUs: rounding mode may be encoded in the instruction
Who is in charge of ensuring the standard?

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- The operating system
- The programming language
  - should have a well-defined semantic
Who is in charge of ensuring the standard?

- The processor
- The operating system
- The programming language
  - should have a well-defined semantic,
  - ... (detailed in some arcane 1000-pages document)
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- The processor
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  - has hundreds of options
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- The **compiler**
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  - some of which to preserve the well-defined semantic of the language
  - but probably **not** by default:
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  - Marketing says: default should be *optimize for speed!*
    - gcc, being free (of the tyranny of marketing), is the safest
    - Commercial compilers compete on the speed of generated code
Who is in charge of ensuring the standard?

- The processor
- The operating system
- The programming language
- The compiler
- The **programmer**
  - ... is in charge in the end.
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So of course, eventually, the programmer will get the blame.
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  - ... is in charge in the end.

So of course, eventually, the programmer will get the blame.

... *or his/her boss.*

Let us educate the programmer.
Processors

Introduction

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Floating-point as it should be: the IEEE-754 standard

Floating-point as it is:

processors,

languages and compilers

Conclusion and perspective
The common denominator of modern processors

- Hardware support for
  - addition/subtraction and multiplication
  - in single-precision (binary32) and double-precision (binary64)
  - SIMD versions: two binary32 operations for one binary64
  - various conversions and memory accesses

- Typical performance:
  - 3-7 cycles for addition and multiplication, pipelined (1 op/cycle)
  - 15-50 cycles for division and square root, not pipelined (hard or soft).
  - 50-500 cycles for elementary functions (soft)
Keep clear from the legacy IA32/x87 FPU

- It is slower than the (more recent) SSE2 FPU
- It is more accurate ("double-extended" 80 bit format), but at the cost of entailing horrible bugs in well-written programs
- the bane of floating-point between 1985 and 2005
A funny horror story

(real story, told by somebody at CERN)

- Use the (robust and tested) standard sort function of the STL C++ library
- to sort objects by their radius: according to $x^2+y^2$.
- Sometimes (rarely) segfault, infinite loop...
- Why?
  - the sort algorithm works under the naive assumption that if $A \not< B$, then $A \geq B$
  - $x^2+y^2$ inlined and compiled differently at two points of the programme,
  - computation on 64 or 80 bits, depending on register allocation
  - enough to break the assumption (horribly rarely).

We will see there was no programming mistake.
And it is very difficult to fix.
The SSEx/AVXy unit of current IA32 processors

- Available for all recent x86 processors (AMD and Intel)
- An additional set of registers, each 128-bit (SSE) or 256-bit (AVX) or 512-bit (AVX-512)
- An additional FP unit able of:
  - 2 / 4 / 8 identical double-precision FP operations in parallel, or
  - 4 / 8 / 16 identical single-precision FP operations in parallel.
- Clean and standard implementation
  - Subnormals trapped to software, or flushed to zero depending on a compiler switch (gcc has the safe default)
- On 64-bit systems, gcc/clang use the SSE instructions by default.
  - To reach for AVX, or downgrade to x87, you need an additional compiler switch
Quickly, the Power family

Power and PowerPC processors, also in IBM mainframes and supercomputers

- No floating-point adders or multipliers
- Instead, one or two FMA: Fused Multiply-and-Add
- Compute $a \times b + c$:
  - faster: roughly in the time of a FP multiplication
  - more accurate: only one rounding instead of 2
  - enables efficient implementation of division and square root

Standardized in IEEE-754-2008 but not yet in your favorite language
Power and PowerPC processors, also in IBM mainframes and supercomputers

- No floating-point adders or multipliers
- Instead, one or two FMA: Fused Multiply-and-Add
- Compute $\circ(a \times b + c)$:
  - faster: roughly in the time of a FP multiplication
  - more accurate: only one rounding instead of 2
  - enables efficient implementation of division and square root
- Standardized in IEEE-754-2008
  - but not yet in your favorite language
Compute $o(a \times b + c)$:
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FMA: the good

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All the modern FPUs are built around the FMA: ARM, Power, IA64, Kalray, all GPGPUs, and even intel from AVX2 and AMD.

enables classical operations, too...

- Addition: $\circ(a \times 1 + c)$
- Multiplication: $\circ(a \times b + 0)$
FMA: ...the bad and the ugly

\[ \circ(a \times b + c) \]

Using it breaks some expected mathematical properties

- Loss of symmetry in \( \sqrt{a^2 + b^2} \)
- Worse: \( a^2 - b^2 \), when \( a = b \):
  \[ \circ( \circ(a \times a) - a \times a ) \]
- Worse: if \( b^2 \geq 4ac \) then (…) \( \sqrt{b^2 - 4ac} \)

Do you see the sort bug lurking?
FMA: ...the bad and the ugly

\( \circ(a \times b + c) \)

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- Worse: if \( b^2 \geq 4ac \) then (...) \( \sqrt{b^2 - 4ac} \)

Do you see the sort bug lurking?

By default, gcc disables the use of FMA altogether
(except as + and \( \times \))
(compiler switches to turn it on)
Languages and compilers

Introduction

Common misconceptions

Floating-point as it should be: the IEEE-754 standard

Floating-point as it is:

processors,

languages and compilers

Conclusion and perspective
Consider the following program, whatever the language:

```c
float a, b, c, d;
x = a + b + c + d;
```

Two questions:
- In which order will the three addition be executed?
- What precision will be used for the intermediate results?
Consider the following program, whatever the language

```c
float a, b, c, d;
x = a + b + c + d;
```

Two questions:

- In which order will the three addition be executed?
- What precision will be used for the intermediate results?

Fortran, C and Java have completely different answers.
float a, b, c, x;
x = a + b + c + d;

- In which order will the three addition be executed?

- With two FPUs (dual FMA, or SSE2, ...),
  
  \((a + b) + (c + d)\) faster than \(((a + b) + c) + d\)
float a, b, c, x;
x = a + b + c + d;

- In which order will the three addition be executed?
  - With two FPUs (dual FMA, or SSE2, ...),
    \((a + b) + (c + d)\) faster than \(((a + b) + c) + d\)
  - If \(a, c, d\) are constants, \((a + c + d) + b\) faster.
float a,b,c,x;
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- In which order will the three addition be executed?
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  - If \(a, c, d\) are constants, \((a + c + d) + b\) faster.
  - (here we should remind that FP addition is not associative
    Consider \(2^{100} + 1 - 2^{100}\))
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- (here we should remind that FP addition is not associative
  
  Consider \(2^{100} + 1 - 2^{100}\))

- Is the order fixed by the language, or is the compiler free to choose?
Evaluation of an expression

float a, b, c, x;

x = a + b + c + d;

- In which order will the three addition be executed?
  - With two FPUs (dual FMA, or SSE2, ...),
    \((a + b) + (c + d)\) faster than \(((a + b) + c) + d\)
  - If \(a, c, d\) are constants, \((a + c + d) + b\) faster.
  - (here we should remind that FP addition is not associative)
    Consider \(2^{100} + 1 - 2^{100}\)
  - Is the order fixed by the language, or is the compiler free to choose?
  - Similar issue: should multiply-additions be fused in FMA?

Florent de Dinechin, Florent.de-Dinechin@insa-lyon.fr  Computing with Floating Point 69
In which order will the three addition be executed?
What precision will be used for the intermediate results?

- **Bottom up** precision: (here all float)
  - context-independent
  - portable
float a, b, c, x;
x = a + b + c + d;

- In which order will the three addition be executed?
- What precision will be used for the intermediate results?
  - *Bottom up* precision: (here all float)
    - context-independent
    - portable
  - Use the maximum precision available which is no slower
    - more accurate result
float a, b, c, x;
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  - Bottom up precision: (here all float)
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    - portable
  - Use the maximum precision available which is no slower
    - more accurate result
  - Is the precision fixed by the language, or is the compiler free to choose?

The FORmula TRANslator translates *mathematical* formula into computations.
Citations are from the Fortran 2000 language standard:

The FORmula TRANslator translates mathematical formula into computations.

Any difference between the values of the expressions \((1./3.)\times3.\) and 1. is a computational difference, not a mathematical difference. The difference between the values of the expressions 5/2 and 5./2. is a mathematical difference, not a computational difference.
Fortran respects mathematics, and only mathematics.

(...) the processor may evaluate any mathematically equivalent expression, provided that the integrity of parentheses is not violated. Two expressions of a numeric type are mathematically equivalent if, for all possible values of their primaries, their mathematical values are equal. However, mathematically equivalent expressions of numeric type may produce different computational results.
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Remark: This philosophy applies to both order and precision.
X, Y, Z of any numerical type, A, B, C of type real or complex, I, J of integer type.

<table>
<thead>
<tr>
<th>Expression</th>
<th>Allowable alternative form</th>
</tr>
</thead>
<tbody>
<tr>
<td>X+Y</td>
<td>Y+X</td>
</tr>
<tr>
<td>X*Y</td>
<td>Y*X</td>
</tr>
<tr>
<td>-X + Y</td>
<td>Y-X</td>
</tr>
<tr>
<td>X+Y+Z</td>
<td>X + (Y + Z)</td>
</tr>
<tr>
<td>X-Y+Z</td>
<td>X - (Y - Z)</td>
</tr>
<tr>
<td>X*A/Z</td>
<td>X * (A / Z)</td>
</tr>
<tr>
<td>X<em>Y-X</em>Z</td>
<td>X * (Y - Z)</td>
</tr>
<tr>
<td>A/B/C</td>
<td>A / (B * C)</td>
</tr>
<tr>
<td>A / 5.0</td>
<td>0.2 * A</td>
</tr>
</tbody>
</table>

Consider the last line:

- A/5.0 is actually more accurate 0.2*A. Why?
- This line is valid if you replace 5 by 4, but not by 3. Why?
Fortunately, Fortran respects your parentheses.

In addition to the parentheses required to establish the desired interpretation, parentheses may be included to restrict the alternative forms that may be used by the processor in the actual evaluation of the expression. This is useful for controlling the magnitude and accuracy of intermediate values developed during the evaluation of an expression.

(this was the solution to the last FP bug of LHC@Home at CERN)
X, Y, Z of any numerical type, A, B, C of type real or complex, I, J of integer type.

<table>
<thead>
<tr>
<th>Expression</th>
<th>Forbidden alternative form</th>
</tr>
</thead>
<tbody>
<tr>
<td>I/2</td>
<td>0.5 * I</td>
</tr>
<tr>
<td>X*I/J</td>
<td>X * (I / J)</td>
</tr>
<tr>
<td>I/J/A</td>
<td>I / (J * A)</td>
</tr>
<tr>
<td>(X + Y) + Z</td>
<td>X + (Y + Z)</td>
</tr>
<tr>
<td>(X * Y) - (X * Z)</td>
<td>X * (Y - Z)</td>
</tr>
<tr>
<td>X * (Y - Z)</td>
<td>X<em>Y-X</em>Z</td>
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</tbody>
</table>
You have been warned.

The inclusion of parentheses may change the mathematical value of an expression. For example, the two expressions $A*I/J$ and $A*(I/J)$ may have different mathematical values if $I$ and $J$ are of type integer.

Difference between $C=(F-32)*(5/9)$ and $C=(F-32)*5/9$. 
Enough standard, the rest is in the manual

(yes, you should read the manual of your favorite language and also that of your favorite compiler)
The C philosophy

The “C99” standard:

*International Standard ISO/IEC 9899:1999(E).*

*Programming languages – C*

- Contrary to Fortran, the standard imposes an order of evaluation
  - Parentheses are always respected,
  - Otherwise, left to right order with usual priorities
  - If you write \( x = \frac{a}{b}/\frac{c}{d} \) (all FP), you get 3 (slow) divisions.

- Consequence: little expressions rewriting
  - Only if the compiler is able to prove that the two expressions always return the same FP number, including in exceptional cases
Morceaux choisis from appendix F.8.2 of the C99 standard:

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- \( x \times 1 \) and \( x / 1 \) may be replaced with \( x \)

However:

- \( x - x \) may not be replaced with \( 0 \)
  - unless the compiler is able to prove that \( x \) will never be \( \infty \) nor \( \text{NaN} \)
- \( x + 0 \) may not be replaced with \( x \)
  - unless the compiler is able to prove that \( x \) will never be \( -0 \)
  - because \((-0) + (+0) = (+0)\) and not \((-0)\)
- On the other hand \( x - 0 \) may be replaced with \( x \)
  - if the compiler is sure that rounding mode will be to nearest.
- \( x == x \) may not be replaced with \( \text{true} \)
  - unless the compiler is able to prove that \( x \) will never be NaN.
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- Worse: $x+0$ may not be replaced with $x$
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Therefore, default behaviour of commercial compiler tend to ignore this part of the standard...
Therefore, **default** behaviour of commercial compiler tend to ignore this part of the standard...
But there is always an option to enable it.
So, perfect determinism wrt order

Strangely, precision is not determined by the standard: it defines a bottom-up minimum precision, but invites the compiler to take the largest precision which is larger than this minimum, and no slower

Idea:

- If you wrote `float` somewhere, you probably did so because you thought it would be faster than `double`.
- If the compiler gives you `long double` you won’t complain.
Drawbacks of C philosophy

- Small drawback
  - Before SSE, float was almost always double or double-extended
  - With SSE, float should be single precision (2-4× faster)
  - Or, on a newer PC, the same computation became much less accurate!

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Computing with Floating Point
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- It does so almost randomly (it totally depends on the context)
- Thus, sometimes a value is rounded twice, which may be even less accurate than the target precision
- And sometimes, the same computation may give different results at different points of the program.
- (sort bug explained when register file is 80 bits and memory storage is 64 bits)
Integrist approach to determinism: *compile once, run everywhere*

- float and double only.
- Evaluation semantics with fixed order and precision.
- No sort bug.
- Performance impact, but...
Quickly, Java

- Integrist approach to **determinism**: *compile once, run everywhere*
  - float and double only.
  - Evaluation semantics with **fixed order and precision**.
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    - Performance impact, but... only on PCs (language designed by Sun when it was selling SPARC)
    - You’ve paid for double-extended processor, and you can’t use it (because it doesn’t *run anywhere*)
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The great Kahan doesn’t like it.
- Many numerical unstabilities are solved by using a larger precision
- Look up *Why Java hurts everybody everywhere* on the Internet

I respectfully disagree with him here. We can’t allow the sort bug.
Floating point numbers

*These represent machine-level double precision floating point numbers. You are at the mercy of the underlying machine architecture (and C or Java implementation) for the accepted range and handling of overflow.*

You have been warned.
Floating point numbers

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You have been warned.

Python does not support single-precision floating point numbers; the savings in processor and memory usage that are usually the reason for using these is dwarfed by the overhead of using objects in Python, so there is no reason to complicate the language with two kinds of floating point numbers.
Conclusion and perspective

Introduction

Common misconceptions

Floating-point as it should be: the IEEE-754 standard

Floating-point as it is:

processors,

languages and compilers

Conclusion and perspective
A historical perspective

Before 1985, floating-point was an ugly mess.

From 1985 to 2000, IEEE-754 becomes pervasive, but the party is spoiled by x87 messy implementation WRT extended precision.

Newer instruction sets solve this problem, but introduce the FMA mess.

In 2008, IEEE 754-2008 cleans up all this, but adds the decimal mess.

and then arrives the multicore mess.
It shouldn’t be so messy, should it?

Don’t worry, things are improving

- SSE2 has cleaned up IA32 floating-point
- Soon (AVX2/SSE5) we have an FMA in virtually any processor and we may use the `fma()` to exploit it portably
- The 2008 revision of IEEE-754 addresses the issues of
  - reproducibility versus performance
  - precision of intermediate computations
  - etc
- but it will take a while to percolate to your programming environment
Tackling the HPC accuracy challenge

Floating point operations are not associative

... but optimisations tend to assume they are (or, that the order is not important):

- blocking for optimal cache usage (ATLAS)
- parallelisation
  - The concept of reduction is valid only for associative operations
- ...

Rationale: there is no reason the new computation order should be worse than the sequential one...
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- blocking for optimal cache usage (ATLAS)
- parallelisation
  - The concept of **reduction** is valid only for associative operations
- ...

Rationale: there is no reason the new computation order should be worse than the sequential one...
Actually there is: the optimizations enable larger problem sizes!
Cooking recipes: If you have to add terms of known different magnitude, it may be a good idea to sort them.

- see the Handbook for variations on this theme
Example: large sums and sums of products

- Cooking recipes: If you have to add terms of known different magnitude, it may be a good idea to sort them
  - see the Handbook for variations on this theme
- Better: bring associativity back by using error-free transformations
Basic EFT blocks

\[ s_h + s_l = a + b \] exactly, and \( s_h = o(a + b) \)

Also 2Mul block: \( p_h + p_l = a \times b \) exactly, and \( p_h = o(a \times b) \)
Theorem (Fast2Sum algorithm)

Assuming

- floating-point in radix $\beta \leq 3$, with subnormal numbers
- correct rounding to nearest
- $a$ and $b$ floating-point numbers
- exponent of $a \geq$ exponent of $b$

The following algorithm computes two floating-point numbers $s$ and $t$ satisfying:

- $s + t = a + b$ exactly;
- $s$ is the floating-point number that is closest to $a + b$.

\[
\begin{align*}
    s &\leftarrow \circ(a + b) \\
    z &\leftarrow \circ(s - a) \\
    t &\leftarrow \circ(b - z)
\end{align*}
\]
Either sort them
  - used to required a branch, which is Very Bad
  - now we have min and max instructions, much better

or use the following

TwoSum

\[
\begin{align*}
  s & \leftarrow o(a + b) \\
  a' & \leftarrow o(s - b), \quad b' \leftarrow o(s - a) \\
  \delta_a & \leftarrow o(a - a'), \quad \delta_b \leftarrow o(b - b') \\
  t & \leftarrow o(\delta_a + \delta_b)
\end{align*}
\]

proven in Coq
  - also works for radix 10
  - even in the presence of underflow

proven minimal branchless algorithm (by enumeration)
Exact product of two FP numbers, with an FMA

\[ r_h \leftarrow (a \times b) \]
\[ r_l \leftarrow (h - a \times b) \]
EFT sum

\[ \sum_{i=1}^{n} s_i = \sum_{i=1}^{n} a_i \text{ exactly} \]

\[ s_n \text{ is the iterative floating-point sum.} \]

No information lost: EFT brings associativity back
A better rule of the game

No information lost: EFT brings associativity back

- Now we can safely play optimization games
- ... with a well-specified rule
- for instance: return correct rounding of the exact sum
- Implementation challenge: compute just right
  (use EFTs only in the degenerate cases that need it)

(about 1 good paper/year on the subject in the last decade)
Example: Compensated sum

Correct the iterative sum with the sum of the “error terms” (the latter being computed naively).

Theorem (Rump, Ogita, and Oishi)

If \( nu < 1 \), then, even in the presence of underflow,

\[
|s - \sum_{i=1}^{n} x_i| \leq u \left| \sum_{i=1}^{n} x_i \right| + \gamma_{n-1}^2 \sum_{i=1}^{n} |x_i|.
\]
error = computed value - reference value

The reference value should **not** be the one computed by the sequential code.

- It is the value defined by the maths (or the physics)

**Example:** the exact sum of $n$ floating-point numbers
(the reference to which sum algorithms should compare)
How accurate is a computation?

\[ \text{error} = \text{computed value} - \text{reference value} \]

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**Example:** the exact sum of \( n \) floating-point numbers

(the reference to which sum algorithms should compare)

**In “real” code, the reference is usually very difficult to define**

- approximation
- discretisation
- rounding
Error analysis

- Proving the absence of over/underflow may be relatively easy
  - when you compute energies, not when you compute areas
Error analysis

- Proving the absence of over/underflow may be relatively easy
  - when you compute energies, not when you compute areas
- Error analysis techniques: how are your equations sensitive to roundoff errors?
  - Forward error analysis: what errors did you make?
  - Backward error analysis: which problem did you solve exactly?

\[
\text{Cond} = \left| \frac{\text{relative change in output}}{\text{relative change in input}} \right| = \lim_{\hat{x} \to x} \frac{|f(\hat{x}) - f(x)|}{f(x)} \cdot \frac{|x - \hat{x}|}{|x|}
\]

\[\text{Cond} \geq 1 \text{ problem is ill-conditioned / sensitive to rounding}\]
\[\text{Cond} \ll 1 \text{ problem is well-conditioned / resistant to rounding}\]

Cond may depend on \(x\): again, make cases...
Error analysis

- Proving the absence of over/underflow may be relatively easy
  - when you compute energies, not when you compute areas
- Error analysis techniques: how are your equations sensitive to roundoff errors?
  - Forward error analysis: what errors did you make?
  - Backward error analysis: which problem did you solve exactly?
- Notion of conditioning:

\[ \text{Cond} = \frac{\text{relative change in output}}{\text{relative change in input}} = \lim_{\hat{x} \to x} \frac{|f(\hat{x}) - f(x)|}{|\hat{x} - x|/x} \]

- \( \text{Cond} \geq 1 \) problem is ill-conditionned / sensitive to rounding
- \( \text{Cond} \ll 1 \) problem is well-conditionned / resistant to rounding
- \( \text{Cond} \) may depend on \( x \): again, make cases...
“Mindless” schemes to improve confidence

- Repeat the computation in arithmetics of increasing precision, until digits of the result agree.
  - Maple, Mathematica, GMP/MPFR

- Repeat the computation with same precision but different (IEEE-754) rounding modes, and compare the results.
  - Easy to do yourself

- Repeat the computation a few times with same precision, rounding each operation randomly, and compare the results.
  - Stochastic arithmetic, CESTAC

- Repeat the computation a few times with same precision but slightly different inputs, and compare the results.

None of these schemes provide any guarantee. They may increase confidence, though.

See “How Futile are Mindless Assessments of Roundoff in Floating-Point Computation ?” on Kahan’s web page
“Mindless” schemes to improve confidence

- Repeat the computation in arithmetics of increasing precision, until digits of the result agree.
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Instead of computing $f(x)$, compute an interval $[f_l, f_u]$ which is guaranteed to contain $f(x)$

- operation by operation
- use directed rounding modes
- several libraries exist

This scheme does provide a guarantee... which is often overly pessimistic ("Your result is in $[-\infty, +\infty]$, guaranteed")

Limit interval bloat by being clever (changing your formula) and/or using bits of arbitrary precision when needed (MPFI library).

Therefore not a mindless scheme
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- Therefore not a mindless scheme
- We have a standard for FP, it is a good one, and eventually your PC will comply
- The standard doesn’t guarantee that the result of your program is close at all to the mathematical result it is supposed to compute.
- But at least it enables serious mathematics with floating-point
So, do you trust your computer now?

“It makes me nervous to fly on airplanes since I know they are designed using floating-point arithmetic.”

A. Householder
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(... well, now they are *piloted* using floating-point arithmetic...)
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Feel nervous, but feel in control.
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Feel nervous, but feel in control.

\textit{It’s not dark magic, it’s science.}
The legacy FPU of IA32 instruction set

Implemented in processors by Intel, AMD, Via/Cyrix, Transmeta... since the Intel 8087 coprocessor in 1985

- internal **double-extended** format on 80 bits:
  - significand on 64 bits, exponent on 15 bits.
- (almost) perfect IEEE compliance on this double-extended format
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- For single and double, IEEE-754-compliant rounding and overflow handling (including exponent) performed when writing back to memory

There probably is a rationale for all this, but... ask Intel people.
Assume you want a portable programme, \( i.e \) use double-precision.

- Fully IEEE-754 compliant possible, but slow:
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  - then write the result of every single operation to memory
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- Next best: compliant except for over/underflow handling:
  - set the status flags to “round significand to 53 bits”
  - but computations will use 15-bit exponents instead of 12
  - OK if if you may prove that your program doesn’t generate huge nor tiny values

- If you compute in registers: register allocation decides if you’re computing on 53 or 64 bits
  - random, unpredictable, unreproducible
  - the bane of floating-point between 1985 and 2005
Computing the area of a triangle

Heron of Alexandria:

\[ A := \sqrt{s(s - x)(s - y)(s - z)} \]
with \( s = (x + y + z)/2 \)
Avoiding cancellations in practice

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Kahan’s algorithm:

Sort \( x, y, z \) so that \( x \geq y \geq z \);

If \( z < x - y \) then no such triangle exists;

else \( A := \sqrt{((x + (y + z)) \times (z - (x - y)) \times (z + (x - y)) \times (x + (y - z))) / 4} \)
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Exercise: solving the quadratic equation by \( \frac{-b \pm \sqrt{b^2 - 4ac}}{2a} \)
Classical example: Muller’s recurrence

\[
\begin{aligned}
  x_0 & = 4 \\
  x_1 & = 4.25 \\
  x_{n+1} & = 108 - \left(815 - \frac{1500}{x_{n-1}}\right)/x_n
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\[
x_n = \frac{\alpha 3^{n+1} + \beta 5^{n+1} + \gamma 100^{n+1}}{\alpha 3^n + \beta 5^n + \gamma 100^n}
\]