Floating-Point Math and Accuracy

Dr. Axel Kohlmeyer

Assistant Dean for High-Performance Computing
Associate Director, ICMS
Associate Director, TMI
College of Science and Technology
Temple University, Philadelphia
axel.kohlmeyer@temple.edu

External Scientific Associate
International Centre for Theoretical Physics, Trieste, Italy
akohlmey@ictp.it

Errors in Scientific Computing

- Before computations:
  - Modeling: neglecting certain properties
  - Empirical data: not every input is known perfectly
  - Previous computations: data may be taken from other (error-prone) numerical methods
  - Sloppy programming (e.g. inconsistent conversions)
- During computations:
  - Truncation: a numerical method approximates a continuous solution
  - Rounding: computers offer only finite precision in representing real numbers

Example

- Computing the surface of the earth using

$$A = 4\pi r^2$$

- This involves several approximations:
  - Modeling: the earth is not exactly a sphere
  - Measurement: earth's radius is an empirical number
  - Truncation: the value of π is truncated
  - Rounding: all numbers used are rounded due to arithmetic operations in the computer
- Total error is the sum of all errors, but one of them is often the dominant error

Representing Numbers (1)

- Real numbers have unlimited accuracy
- Yet computers "think" digital, i.e. in integer math
  => only a fixed **range** of numbers can be
  represented by a fixed number of bits
  => **distance** between two integers is 1
- We can reduce the distance through fractions (= fixed point), but that also reduces the range

	16-bit	32-bit	64-bit	28-bit / 4-bit	22-bit / 10-bit
Min.	-32768	-2147483648	~ $-9.2233 * 10^{-18}$	-16777216.0000	-2048.000000
Max.	32767	2147483647	~ $9.2233 * 10^{-18}$	16777215.9375	~ 2047.999023
Dist.	1	1	1	0.0635	0.0009765625

Representing Numbers (2)

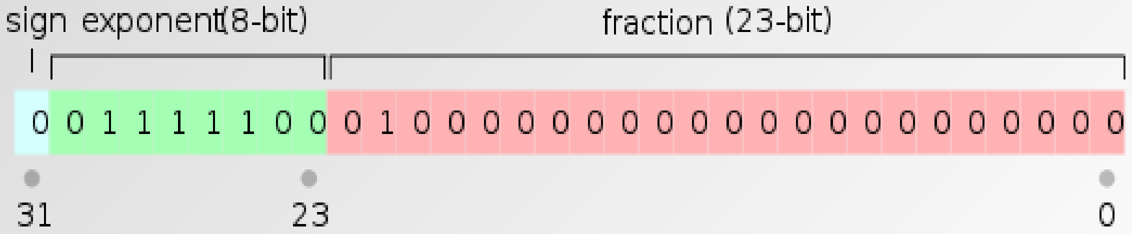
- Need a way to represent a wider range of numbers with a same number of bits
- Need a way to represent numbers with a reasonable amount of precision (distance)
- Same relative precision often sufficient:

  => Scientific notation:
  $$+/-(\text{mantissa}) * (\text{base})^{+/-(\text{exponent})}$$

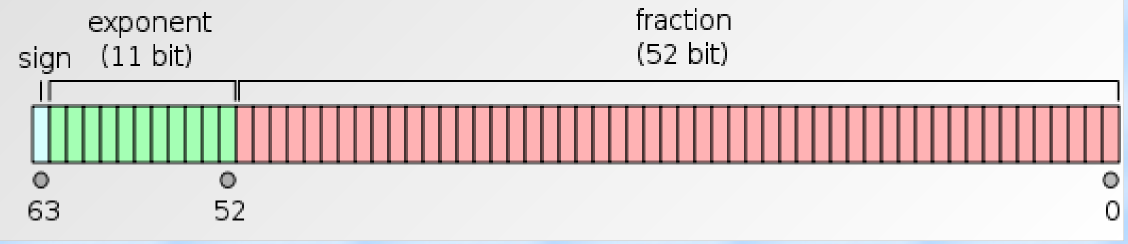
  Mantissa -> integer fraction
  Base -> 2
  Exponent -> a small integer

IEEE 754 Floating-point Numbers

- The IEEE 754 standard defines: storage format, result of operations, special values (infinity, overflow, invalid number), error handling
  => portability of compute kernels ensured
- Numbers are defined as bit patterns with a sign bit, an exponential field, and a fraction field
  - Single precision:
    8-bit exponent
    23-bit fraction



  - Double precision:
    11-bit exponent
    52-bit fraction



Values of Floating-Point Numbers

- Value: $(1 – (\text{mantissa})/(2^{(\text{fraction bits})}) * 2^{(\text{exponent-bias})}$
  $1.0 \leq (\text{mantissa}) < 2.0$, $(\text{exponent}) \geq 0$
- Special case: 0.0 is all bits set to zero
  Special case: -0.0 is like 0.0 but sign bit is set
  More special cases: Inf, -Inf, NaN, -NaN
- Single precision: $\sim\pm1.2*10^{-38} < x < \sim\pm3.4*10^{38}$
  actual precision: ~7 decimal digits
- Double precision: $\sim\pm2.2*10^{-308} < x < \sim\pm1.8*10^{308}$
  actual precision: ~15 decimal digits

Density of Floating-point Numbers

- How can we represent so many more numbers in floating point than in integer? ***We don't!***
- The number of unique bit patterns has to be the same as with integers of the same bitness
- There are 8,388,607 single precision numbers in $1.0 < x < 2.0$, but only 8191 in $1023.0 < x < 1024.0$
- => absolute precision depends on the magnitude
- => some numbers are not represented exactly => approximated using rounding mode (nearest)

Math with Floating Point Numbers

Addition:

- Right bitshift mantissa and increment exponent of smaller number until both exponents are the same
- Add mantissa of both numbers and bitshift until mantissa is between 1.0 and 2.0 again
- Only if both numbers have the same sign and the same exponent precision is preserved

Multiplication:

- Add exponents and multiply mantissa of both numbers
- Bitshift mantissa until its value is between 1.0 and 2.0
- No loss of precision; error is larger error of either number

Floating-Point Math Pitfalls

- Floating point math is commutative,
  but <u>not associative</u>! Example (single precision):
  $1.0 + (1.5*10^{38} + (- 1.5*10^{38})) = 1.0$
  $(1.0 + 1.5*10^{38}) + (- 1.5*10^{38}) = 0.0$
- => the result of a summation depends on the order of how the numbers are summed up
- => results may change significantly, if a compiler changes the order of operations for optimization
- => prefer adding numbers of same magnitude
  => avoid subtracting very similar numbers

How To Reduce Errors

- Use double precision unless you can be sure of error cancellation or using an imprecise model => collides with vectorization and GPU/MIC
- When summing numbers of different magnitude
  - Sort first and sum in ascending order
  - Sum in blocks (pairs) and then sum the sums
  - Use integer fraction, if range and precision allow it
- NOTE: summing numbers in parallel may give different results depending on parallelization

Floating Point Comparison

- Floating-point results are usually **inexact**
  => comparing for equality is dangerous
  Example: don't use a floating point number for controlling a loop count. Integers are made for it
- It is OK to use exact comparison:
  - When results have to be bitwise identical
  - To prevent division by zero errors
- => compare against expected absolute error
- => don't expect higher accuracy than possible

Floating Point vs. Math Library

- libm is part of standard C, thus it is ubiquitous
- Provides a large variety of mathematical functions / operations on floating-point numbers but not many alternatives for x86/x86_64 exist
- Focus is typically put on standard compliance
- The x86 floating point unit contains most of the functionality internally, but most as firmware; SSE and AVX do not provide these
- The x86 FPU log() is slower than GNU libm

Test Examples (1)

- **`inverse`**: computes *y=1/x* and *z=x*y* and checks if the result is exactly 1.0.
  Compare compilation using `gfortran -O2` and `gfortran -O2 -ffast-math`
- **`loop`**: advance x from 0.0 to 1.0 in increments of 0.01. Compare looping over integer and real
- **`epsilon`**: determine the floating-point precision through searching for the largest epsilon for which 1.0 + ε == 1.0. Start with ε = 1.0 and repeatedly dividing by 2.0

Test Examples (2)

- **`sum_number`**: compare summing accuracy depending on ascending or descending order. Find the smallest N where the sums differ
- **`paranoia`**: IEEE-754 compliance test
=> use `make` to compile with different compiler flags for optimization and math accuracy
- **`mathopt`**: compute windowed average with a two and three numbers wide window.
=> speed of division by 2 vs division by 3
=> impact of compiler flags vs. code rewrite

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axel.kohlmeyer@temple.edu

External Scientific Associate
International Centre for Theoretical Physics, Trieste, Italy
akohlmey@ictp.it