#### **Floating-Point Math and Accuracy**

### Dr. Axel Kohlmeyer

Research Professor, Department of Chemistry
Associate Director, ICMS
College of Science and Technology
Temple University, Philadelphia
axel.kohlmeyer@temple.edu



## 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  $\pi$  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 <u>range</u> 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 <sup>-18</sup>	-16777216.0000	-2048.000000
Max.	32767	2147483647	~ 9.2233 * 10 <sup>-18</sup>	16777215.9375	~ 2047.999023
Dist.	1	1	1	0.0635	0.0009765625



# Representing Numbers (2)

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

```
=> Scientific notation:
+/-(mantissa) * (base) */-(exponent)
```

Mantissa -> integer fraction

Base -> 2

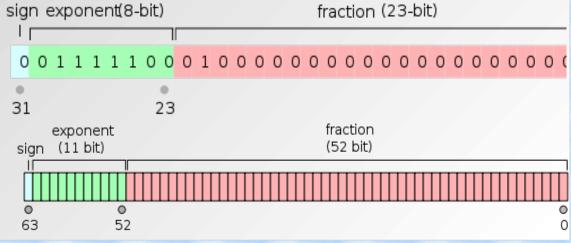
Exponent -> a small integer



### 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 exponent23-bit fraction
  - Double precision:11-bit exponent52-bit fraction

Master in High Performance Computing



## Values of Floating-Point Numbers

- Value:  $(1 (mantissa)/(2^{(fraction bits)}) * 2^{(exponent-bias)}$  $1.0 \le (mantissa) < 2.0, (exponent) \ge 0$
- 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:  $\sim \pm 1.2*10^{-38} < x < \sim \pm 3.4*10^{38}$  actual precision:  $\sim 7$  decimal digits
- Double precision: ~ $\pm 2.2*10^{-308}$  < x < ~ $\pm 1.8*10^{308}$  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 <u>has</u> to be the <u>same</u> 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 <u>have</u> 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



#### More Information on the Web

- https://blog.reverberate.org/2014/09/whatevery-computer-programmer-should.html
- https://blog.reverberate.org/2016/02/06/floatingpoint-demystified-part2.html
- https://floating-point-gui.de/



# 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 -02 and gfortran -02 -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 +  $\epsilon$  == 1.0. Start with  $\epsilon$  = 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

