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Second Computational and Data Science school for HEP (CoDaS-HEP)

### SETUP – EXAMPLES / EXERCISES

- Prerequisites:
  - Recent C++ compiler (at least C++11 compliant)
  - Eventually CMake
- git clone https://github.com/mpbl/codas\_fpa/
- README.md for instructions



### OUTLINE

#### Disasters

- Reminder on integers
- Floating point numbers
- IEEE 754
  - Rounding modes, exceptions, underflow, ...
- Improving FPA accuracy
  - Kahan algorithm, FMA
- Computing Faster
  - Fast Math, reduced precision, mixed precision
- Concurrency
- Conclusion
- References



### DISASTERS DUE TO MACHINE REPRESENTATION

#### **Patriot Missile Failure**

#### **Rounding errors**

1991, Gulf War. Failed to track and intercept an incoming Iraqi Scud missile. Inaccurate calculation of the time since boot due to computer arithmetic errors



Explosion of the Ariane 5 Overflow 1996, Kourou, French Guiana software error in the inertial reference system Storing 64 bits FP into 16 bits integers



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http://www-users.math.umn.edu/~arnold/disasters/

# A WORD ABOUT INTEGERS

```
template <typename Integer>
void world_population() {
    //
https://en.wikipedia.org/wiki/List_of_continents_by_population
    // in 2010
    std::cout << "Sizeof(Integer) : " << sizeof(Integer) <<
std::endl;</pre>
```

```
01_integer/integer_overflow
```

- How many people, worldwide?
- Does it makes sense?
- What might be the problem?
- Why data are from 2010 and not 2016?



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world\_population<uint32\_t>();

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}

### **REMINDER: INTEGERS**

- ➔ int is not integer
- Representation uses a limited number of bits
  - Positive numbers are just represented using their binary form
  - Negative numbers often use two's complement
- Properties of arithmetic types can be queried using std::numeric\_limits (C++)
  - On my machine (and probably on yours)
    - $2^{32} < int = int32_t <= 2^{31}-1$  // 1 bit is used to store the sign
    - $0 < unsigned int = uint32_t <= 2^{32}$



### WHY USING FLOATING POINT NUMBERS

- Representing numbers that would be too large or too small to be represented as integers
  - 1.4e-45 to 3.4e38
- Representing numbers that are not representable as integers
- Of course, floating points representations are also subject to use only a limited number of bits.



# DESIRABLE PROPERTIES

- Speed
- Accuracy:
  - "Correct" results
- Range:
  - Large and small numbers
- Portability:
  - Run on different machines, giving the same answer
- Ease of implementation and use
  - Needs to feel natural, at least to the user



## REAL TO FLOATING POINTS

• A number is represented exactly by: Significand × base<sup>exponent</sup>

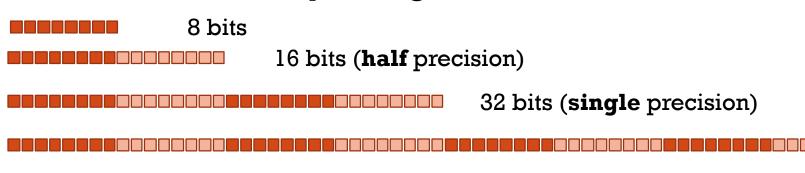
By instance:

 $3.1415 = 31415 \times 10^{-4}$ 

Significand:

- Mantissa
- Coefficient Base:
- Radix

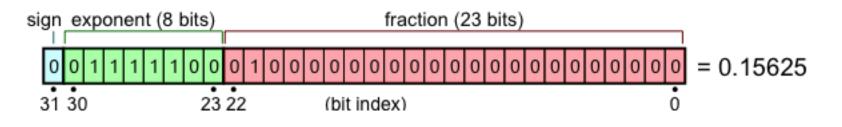
Stored in memory using a limited number of bits:



64 bits (double precision)



### IEEE 754 REPRESENTATION OF SINGLE PRECISION FP

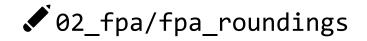


Exponent	Fraction == 0	Fraction != 0	Equation
All Zeros	0, -0	Subnormal value (Fraction starts with an implicit 0)	(-1) <sup>sign</sup> × 2 <sup>-126</sup> × 0.fraction
All Ones	<u>+</u> ∞	NaN	
Otherwise	Normalized value (Fraction starts with an implicit 1)		$(-1)^{sign} \times 2^{exponent - 127} \times 1.$ fraction

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https://en.wikipedia.org/wiki/Single-precision\_floating-point\_format





### ROUNDING MODES

#### Roundings to nearest

- Round to nearest, ties to even [Default Mode] rounds to the nearest value; if the number falls midway it is rounded to the nearest value with an even (zero) least significant bit; this is the default for binary floating-point and the recommended default for decimal.
- Round to nearest, ties away from zero rounds to the nearest value; if the number falls midway it is rounded to the nearest value above (for positive numbers) or below (for negative numbers); this is intended as an option for decimal floating point.

#### Directed roundings

- Round toward 0 directed rounding towards zero (also known as truncation).
- Round toward +∞ directed rounding towards positive infinity (also known as rounding up or ceiling).
- Round toward -∞ directed rounding towards negative infinity (also known as rounding down or floor).



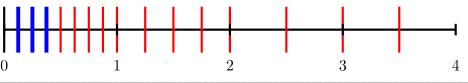
## FLOATING POINT EXCEPTIONS

- The IEEE standard defines several FP exceptions
  - Can be ignored  $\rightarrow$  Default action is taken
  - Can be trapped 
     Error is signaled
- **Underflow**: Too small to be represented as a normalized float in its format.
  - If ignored, the operation results in a denormalized float or zero.
- **Overflow**: Too large to be represented as a float in its format.
  - If ignored, the operation results in the appropriate infinity.
- Divide-by-zero: Float is divided by zero.
  - If ignored, the appropriate infinity is returned.
- **Invalid**: Ill-defined operation, such as (0.0/ 0.0).
  - If ignored, a quiet NaN is returned.
- Inexact: The result of a floating point operation is not exact, i.e. the result was rounded.
  - If ignored, the rounded result is returned CoDaS-HEP



## GRADUAL UNDERFLOW (SUBNORMALS)

- Subnormals (or denormals) are FP smaller than the smallest normalized FP: they have leading zeros in the significand
  - For single precision they represent the range 10<sup>-38</sup> to 10<sup>-45</sup>



- Subnormals guarantee that additions never underflow
  - Any other operation producing a subnormal will raise a underflow exception if also inexact
- Hardware is not always able to deal with subnormals
  - Software assist is required: SLOW
  - To get correct results even the software algorithms need to be specialized

It is possible to tell the hardware to flush-to-zero (ftz) subnormals
 It will raise underflow and inexact exceptions

13

### IMPROVED ACCURACY: KAHAN SUMMATION ALGORITHM

```
function KahanSum(input)
    var sum = 0.0
    var c = 0.0 // A running compensation for lost low-order bits.
    for i = 1 to input.length do
        var y = input[i] - c // So far, so good: c is zero.
       // Alas, sum is big, y small, so low-order digits of y are lost.
        var t = sum + y
        // (t - sum) cancels the high-order part of y;
        // subtracting y recovers negative (low part of y)
        // Algebraically, c should always be zero.
        // Beware overly-aggressive optimizing compilers!
        c = (t - sum) - y
       sum = t
    return sum
                                             patriot/patriot.cpp (V. Innnocente)
```

https://en.wikipedia.org/wiki/Kahan\_summation\_algorithm

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### IMPROVED ACCURARY

- Kahan Summation Algorithm does not work for "ill-conditioned" sums
  - In particular in an element is larger than the sum
- Other summation algorithms
  - Fast2Sum (Dekker), 2Sum (Knuth et al.), ...
- Products also have specific algorithms for accurate computations:
  - Dekker, ...
- Algorithms for computing means, variances, …

### Ber Handbook of Floating-Point Arithmetic



### FUSED MULTIPLY-ACCUMULATE (FMA)

- Or Fused Multiply-Add (FMA) :  $a \times b + c$
- Multiplier–Accumulator (MAC) hardware unit
- Performed with a single rounding (<u>IEEE 754-2008</u>) (instead of 2 for one multiplication followed by an addition)
- A fast FMA can speed up and improve the accuracy of many computations that involve the accumulation of products:
  - Dot product
  - Matrix multiplication
  - Polynomial evaluation (e.g., with Horner's rule)
  - Newton's method for evaluating functions.
  - Convolutions and artificial neural networks

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https://en.wikipedia.org/wiki/Multiply%E2%80%93accumulate\_operation

# **ROUND-OFF ERROR ANALYSIS**

### Inverse analysis

 based on the "Wilkinson principle": the computed solution is assumed to be the exact solution of a nearby problem provides error bounds for the computed results

### Interval arithmetic

- The result of an operation between two intervals contains all values that can be obtained by performing this operation on elements from each interval.
  - guaranteed bounds for each computed result
  - the error may be overestimated
  - specific algorithms

### Probabilistic approach

- uses a random rounding mode
- estimates the number of exact significant digits of any computed result

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http://www.math.twcu.ac.jp/~conf/FJWNC2015/doc/Jezequel.pdf



# COST OF OPERATIONS (IN CPU CYCLES)

Operator	Instruction	AVX FP32	AVX FP64
+,-	ADD, SUB	3	3
==,!=	COMISS, CMP	2,3	2,3
cast fp32 <-> fp64	CVT	4	4
,&,^	AND, OR	1	1
*	MUL	5	5
/, sqrt	DIV, SQRT	21-29	21-45
l.f/□, l.f/sqrt□	RCP, RSQRT	7	
=	MOV	1,4	1,4



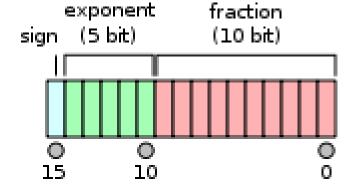
### FAST MATH

- man gcc /-ffast-math -- Sets the options:
- -fno-math-errno
  - Do not set "errno" after calling math functions that are executed with a single instruction
- -funsafe-math-optimizations :
  - assume that arguments and results are valid.
- -ffinite-math-only
  - Allow re-association of operands in series of floating-point operations.
  - Patriot example ?
- -fno-rounding-math
  - Disable transformations and optimizations that assume default floating-point rounding behavior.
- -fno-signaling-nans
  - Do not assuming that IEEE signaling NaNs may generate user-visible traps during floating-point operations. (default)
- -fcx-limited-range: range check for complex division.

## SPEEDING MATH UP

- Avoid or factorize-out division and sqrt
  - if possible compile with "–Ofast" or "-ffast-math"
- Prefer linear algebra to trigonometric functions
- Cache quantities often used
  - No free lunch: at best trading memory for cpu
- Choose precision to match required accuracy
  - Square and square-root decrease precision
  - Catastrophic precision-loss in the subtraction of almost-equal large numbers

### HALF PRECISION

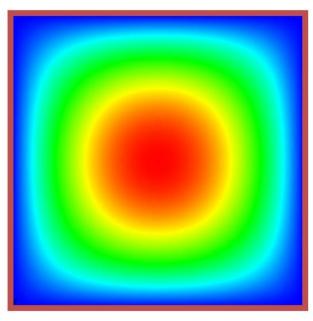


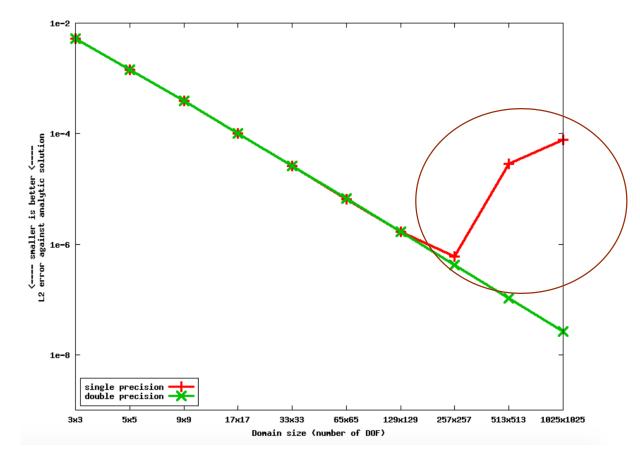
- Getting popular for some machine learning application
  - NVIDIA P100 can perform FP16 arithmetic at twice the throughput of FP32.
- Large number of parameters and the generally modest accuracy required for the final output – is this image a cat? or is this a fraudulent application?
- Training can be successful with floating point half precision (16 bits) or with fixed point or integers (as low as 8 bits in some cases).
- Don't use it blindly in your codes: Check first!



### SINGLE VS. DOUBLE PRECISION

- For some problem it does matter
- Poisson Equation  $-\Delta u = f$ 
  - Finite elements





#### Strzodka et al.

http://www.nvidia.com/content/nvision2008/tech\_presentations/ 7/25/18 NVIDIA\_Research\_Summit/NVISION08-Mixed\_Precision\_Methods\_on\_GPUs.pdf

Strzodka et al. <u>http://www.nvidia.com/content/nvision2008/tech\_presentations/</u> NVIDIA\_Research\_Summit/NVISION08-Mixed\_Precision\_Methods\_on\_GPUs.pdf

### MIXED-PRECISION

- Exploit the speed of low precision and obtain a result of high accuracy  $d_k = b Ax_k$ 
  - Compute in high precision (cheap)
  - Solve in low precision (fast)
  - Correct in high precision (cheap)
  - Iterate until convergence in high precision

$$d_{k} = b-Ax_{k}$$
$$Ac_{k} = d_{k}$$
$$x_{k+1} = x_{k}+c_{k}$$
$$k = k+1$$

- Now also half-precision in single precision codes
  - <u>https://devblogs.nvidia.com/parallelforall/mixed-precision-programming-cuda-8/</u>

### CONCURRENCY

Concurrency makes it worse!

- Operations a shared variables (e.g. reduction)
- Concurrency implies unknown orders for operation
- Inherent to concurrency; does not depend on the parallel model
- Worst as the degree of parallelism increases
  For instance, on GPU codes using atomics



### CONCLUSION

Should you worry about the accuracy of every LoC you write?

- Study your problem /algorithm to understand what level of precision is required / acceptable
  - Usually the answer is already known by your community
- Verify your results / programs
  - Convergence tests, statistical tests, analytical solutions, …
- Check for performance bottlenecks
  - Other CoDaS' talks

### REFERENCES

- Optimal floating point computation: Accuracy, Precision, Speed in scientific computing. Innocente. 2012
- Handbook of Floating-Point Arithmetic. Mueller et al. 2010
- What Every Computer Scientist Should Know About Floating-Point Arithmetic. Goldberg. https://docs.oracle.com/cd/E19957-01/806-3568/ncg\_goldberg.html

