Numerics

Ramses van Zon

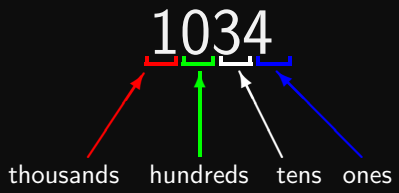
PHY1610, Winter 2025

Numbers


SciNet
ADVANCED RESEARCH COMPUTING at the UNIVERSITY OF TORONTO

How do we represent quantities?

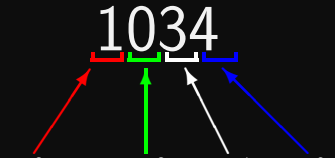
- We use numbers, of course.
- In grade school we are taught that numbers are organized in columns of digits. We learn the names of these columns.
- The numbers are understood as multiplying the digit in the column by the number that names the column.



$$1034 = (1 \times 1000) + (0 \times 100) + (3 \times 10) + (4 \times 1)$$

Other ways to represent a quantity

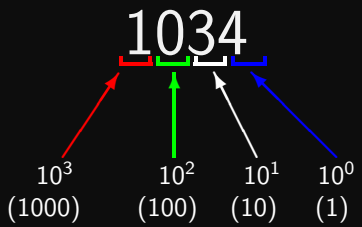
- Instead of using ‘tens’ and ‘hundreds’, let’s represent the columns by powers of what we will call the ‘base’.
- Our normal way of representing numbers is ‘base 10’, also called decimal.
- Each column represents a power of ten, and the coefficient can be one of 10 numerals (0-9).

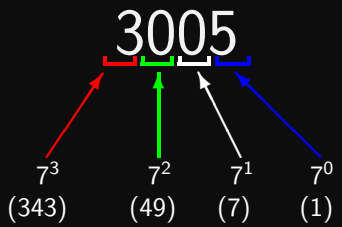


$$1034 = (1 \times 10^3) + (0 \times 10^2) + (3 \times 10^1) + (4 \times 10^0)$$

You can choose any base you want

How do we represent the quantity 1034 if we change bases? What about base 7 (septenary)?





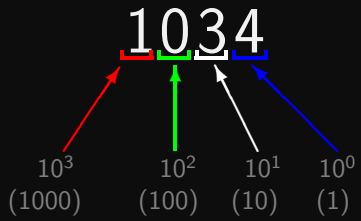
$$1034 = (1 \times 10^3) + (0 \times 10^2) + (3 \times 10^1) + (4 \times 10^0)$$

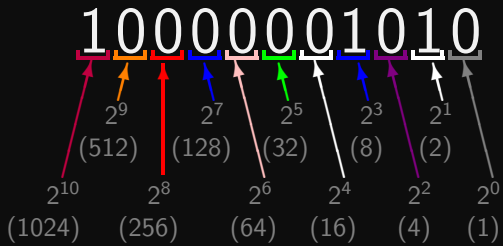
$$1034 = (3 \times 7^3) + (0 \times 7^2) + (0 \times 7^1) + (5 \times 7^0)$$

In base 7 the numerals have the range 0-6.

Who cares?

The reason we care is because computers do not use base 10 to store their data. Computers use base 2 (binary). The numerals have the range 0-1.





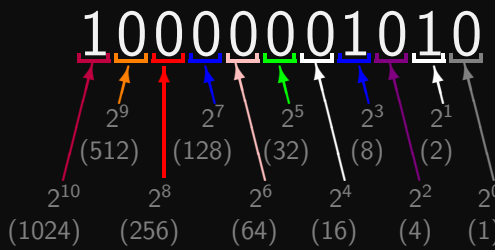
$$1034 = (1 \times 10^3) + (0 \times 10^2) + (3 \times 10^1) + (4 \times 10^0)$$

$$\begin{aligned} 1034 \;=\; & (1 \times 2^{10}) + (0 \times 2^9) + (0 \times 2^8) + (0 \times 2^7) \\ & + (0 \times 2^6) + (0 \times 2^5) + (0 \times 2^4) + (1 \times 2^3) \\ & + (0 \times 2^2) + (1 \times 2^1) + (0 \times 2^0) \end{aligned}$$

Why do computers use binary numbers?

Why use binary?

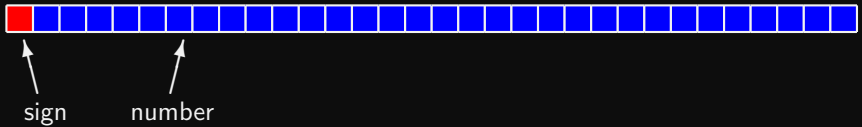
- Modern computers operate using circuits that have one of two states: ‘on’ or ‘off’.
- This choice is related to the complexity and cost of building binary versus ternary circuitry.
- Binary numbers are like series of ‘switches’: each digit is either ‘on’ or ‘off’.
- Each ‘switch’ in the number is called a ‘bit’.



Finite Binary Representations of Numeric Types

Integers

- All integers are exactly representable.
- Different sizes of integer variables are available, depending on your hardware, OS, and programming language.
- For most languages, a typical integer is 32 bits,
- 1 bit for the sign, which, when set, subtracts 2^{32} of the number.
- Finite range: can go from -2^{31} to $2^{31} - 1$ (-2,147,483,648 to 2,147,483,647).
- Unsigned integers: $0 \ldots 2^{32} - 1$.
- All operations ($+$, -, *) between representable integers are represented unless there is overflow.



A typical int = 32 bits = 4 bytes.

Long integers

- Long integers are like regular integers, just with a bigger memory size, usually 64 bits.
- And consequently a bigger range of numbers.

- One bit for sign.
  (when set, subtracts 2^{64} of the number)
- Can go from -2^{63} to $2^{63} - 1$
  (-9,223,372,036,854,775,808 to 9,223,372,036,854,775,807)
- Unsigned long integers: $0 \ldots 2^{64} - 1$.

A typical long int = 64 bits = 8 bytes.

Integers in C++

Type	Typical size (Linux x86_64)
char	1 byte
short	2 bytes
int	4 bytes
long	8 bytes
long long	8 bytes

Size/Type	Range
1 byte signed	-128 .. 127
1 byte unsigned	0 .. 255
2 byte signed	-32,768 .. 32,767
2 byte unsigned	0 .. 65,535
4 byte signed	-2,147,483,648...2,147,483,647
4 byte unsigned	0 .. 4,294,967,295
8 byte signed	-9,223,372,036,854,775,808 .. 9,223,372,036,854,775,807
8 byte unsigned	0..18,446,744,073,709,551,615

```
char c;
short int si;        // valid
short s;             // preferred
int i;
long int li;         // valid
long l;              // preferred
long long int lli;   // valid
long long ll;        // preferred
signed char c;
signed short s;      // unnecessary
signed int i;        // unnecessary
signed long l;       // unnecessary
signed long long ll;// unnecessary
unsigned char c;
unsigned short s;
unsigned int i;
unsigned long l;
unsigned long long ll;
```

Integers in C++, practically

Type	Size
char	1 byte
int16_t	2 bytes
int32_t	4 bytes
int64_t	8 bytes
int	at least 2 bytes, usually 4
long long	at least 8 bytes
size_t	unsigned, to represent memory size

Size/Type	Range
1 byte signed	-128 .. 127
1 byte unsigned	0 .. 255
2 byte signed	-32,768 .. 32,767
2 byte unsigned	0 .. 65,535
4 byte signed	-2,147,483,648...2,147,483,647
4 byte unsigned	0 .. 4,294,967,295
8 byte signed	-9,223,372,036,854,775,808 .. 9,223,372,036,854,775,807
8 byte unsigned	0..18,446,744,073,709,551,615

```cpp
#include <cstddef>
#include <cstdint>
//...
  char           c;  //  *is* a byte
  signed char    sc;
  int16_t        ssi;
  int32_t        sni;
  int62_t        sli;
  int            si;  // used in libraries
  long long      sli;
  unsigned char uc;
  uint16_t       usi;
  uint32_t       uni;
  uint64_t       uli;
  unsigned       ui;
  size_t         uli; // used in libraries
```

Integer OverFlow

```cpp
#include <iostream>
#include <cstdint>

int main()
{
    uint16_t x = 65535; // largest 16-bit unsigned value possible
    std::cout << "x was: " << x << "\n";
    x++; // 65536 is out of our range -- we get overflow because x can't hold 17 bits
    std::cout << "x is now: " << x << "\n";
    return 0;
}
```

```
$ g++ -std=c++17 int_exampleOF1.cpp
$ ./a.out
x was: 65535
x is now: 0
```

```cpp
#include <iostream>
#include <cstdint>

int main()
{
    uint16_t x = 0; // smallest 2-byte unsigned value possible
    std::cout << "x was: " << x << "\n";
    x--; // overflow!
    std::cout << "x is now: " << x << "\n";
    return 0;
}
```

```
$ g++ -std=c++17 int_exampleOF2.cpp
$ ./a.out
x was: 0
x is now: 65535
```

Fixed point numbers

How do we deal with decimal places?

- We could treat real numbers like integers: 0 . . . INT_MAX, and only keep, say, the last two digits behind the decimal point.
- This is known as 'fixed point' numbers, since the decimal place is always in the same spot.
- This is often used for financial timeseries data, since they only use a finite number of decimal places.
- But this is terrible for scientific computing. Relative precision varies with magnitude; we need to be able to represent small and large numbers at the same time.

Floating point numbers

Floating point numbers

- Analog of numbers in scientific notation.
- Of course, using binary, not decimal.
- Inclusion of an exponent means the decimal/binary point is 'floating'.
- One bit is dedicated to sign.
- By "normalizing", the part before the binary point can always be made 1.

$$-\ 1.34 \times 10^{-7}$$

sign mantissa base exponent

A single precision real = 32 bits = 4 bytes.
A double precision real = 64 bits = 8 bytes.

Floats in C++

Type	Size	Mantissa	Exponer
(float16_t)	2 bytes	10	5
float	4 bytes	23	8
double	8 bytes	52	11
long double	8/12/16 bytes	?	?

```
float fValue;
double dValue;
long double dValue2;

int n(5); // 5 means integer
double d(5.0); // 5.0 means fp (double by default)
float f(5.0f); // 5.0 means fp, f suffix means float

double d1(5000.0);
double d2(5e3); // another way to assign 5000
double d3(0.05);
double d4(5e-2); // another way to assign 0.05
```

Virtually all CPUs and GPUs have native support for working with floats and doubles in hardware.

Many GPUs have 16bit float support.

Without native support, floating point operations have to be emulated and are slow.

Size/Type	Range	Precision
4 bytes	$\pm 1.18 \times 10^{-38}$ to $\pm 3.4 \times 10^{38}$	6-9 sign.digits, typically 7
8 bytes	$\pm 2.23 \times 10^{-308}$ to $\pm 1.80 \times 10^{308}$	15-18 sign.digits, typ. 16
12 bytes	$\pm 3.65 \times 10^{-4951}$ to $\pm 1.18 \times 10^{4932}$	18-21 significant digits
16 bytes	$\pm 3.36 \times 10^{-4932}$ to $\pm 1.18 \times 10^{4932}$	33-36 significant digits

Special ‘numbers’ & Numeric Limits Interface

Special numbers

This format for storing floating point numbers comes from the IEEE 754 standard.

There's room in the format for the storing of a few special numbers.

- Signed infinities **(+Inf, -Inf)**: result of overflow, or divide by zero.
- Signed zeros: signed underflow, or divide by $+/-$**Inf**.
- Not a Number (**NaN**): square root of a negative number, 0/0, Inf/Inf, *etc.*
- The events which lead to these are usually errors, and can be made to cause exceptions.

#include <limits>

```
template<class T> class numeric_limits<T>;
class numeric_limits<char>;
class numeric_limits<signed char>;
class numeric_limits<unsigned char>;
class numeric_limits<short>;
class numeric_limits<unsigned short>;
class numeric_limits<int>;
class numeric_limits<unsigned>;
```

```
class numeric_limits<long>;
class numeric_limits<unsigned long>;
class numeric_limits<long long>;
class numeric_limits<unsigned long long>;
class numeric_limits<float>;
class numeric_limits<double>;
class numeric_limits<long double>;
```

Member Functions

`min()`	returns the smallest finite value of the given type
`lowest()`	returns the lowest finite value of the given type
`max()`	returns the largest finite value of the given type
`epsilon()`	returns the difference between 1.0 and the next representable value of the given flo
`round_error()`	returns the maximum rounding error of the given floating-point type
`infinity()`	returns the positive infinity value of the given floating-point type
`quiet_NaN()`	returns a quiet NaN value of the given floating-point type
`signaling_NaN()`	returns a signaling NaN value of the given floating-point type
`denorm_min()`	returns the smallest positive subnormal value

C++ Numeric Limits – example

```cpp
#include <limits>
#include <iostream>

int main()
{
    std::cout << "type\tlowest\thighest\n";
    std::cout << "int\t"
              << std::numeric_limits<int>::lowest() << '\t'
              << std::numeric_limits<int>::max() << '\n';
    std::cout << "float\t"
              << std::numeric_limits<float>::lowest() << '\t'
              << std::numeric_limits<float>::max() << '\n';
    std::cout << "double\t"
              << std::numeric_limits<double>::lowest() << '\t'
              << std::numeric_limits<double>::max() << '\n';
}
```

```
$ g++ -std=c++17 limits.cpp
$ ./a.out
type    lowest          highest
int     -2147483648     2147483647
float   -3.40282e+38    3.40282e+38
double  -1.79769e+308   1.79769e+308
```

IEEE-754/854 Standards

`float` (single precision real) = 32 bits = 4 bytes $\rightsquigarrow$ IEEE-754

`double` (double precision real) = 64 bits = 8 bytes $\rightsquigarrow$ IEEE-854

Property	Value for float	Value for double
Largest rep.nbr.	3.402823466e+38	1.7976931348623157e+308
Smallest nbr. without losing precision	1.175494351e-38	2.2250738585072014e-308
Smallest rep.nbr.	1.401298464e-45	5e-324
Mantissa bits	23	52
Exponent bits	8	11
Epsilon	1.1929093e-7	2.220446049250313e-16

Limitations in floating point mathematics

There are limitiations inherent in using finite-length floating point variables.

- Except for numbers that fit exactly into a base two representation, assigning a real number to a floating point variable involves truncation.
- Think about how you represent 1/3. Is it 0.3? 0.33? 0.333?
- You end up with an error of 1/2 ULP
  (Unit in Last Place)

Unrepresentable numbers

In base two, 0.1 is an infinitely repeating fraction: $0.0001100110011001100110011\ldots$

So this cannot be represented exactly in finite binary!

Limited accuracy

Single precision: 1 part in $2^{-24} \sim$ 6e-8.
Double precision: 1 part in $2^{-53} \sim$ 1e-16.

Aside: want to see more digits in output?

```cpp
#include <iostream>
#include <iomanip>

void output(float f, double d) {
  std::cout << "f = " << f << '\n';
  std::cout << "d = " << d << '\n';
  std::cout << "f+d = " << f+d << '\n';
  std::cout << "f-d = " << f-d << '\n';
  std::cout << "f*d = " << f*d << '\n';
  std::cout << "f/d = " << f/d << '\n';
  std::cout << "d/f = " << d/f << '\n';
}

int main()
{
  output(0.01f, 1.0e-17);
  // set fixed floating format
  std::cout.setf(std::ios::fixed);
  // change fixed format precision
  std::cout.precision(5);
  //
  output(0.01f, 1.0e-17);
}
```

```
$ g++ -std=c++17 fp_ariths.cpp
$ ./a.out
f = 0.01
d = 1e-17
f+d = 0.01
f-d = 0.01
f*d = 1e-19
f/d = 1e+15
d/f = 1e-15

f = 0.01000
d = 0.00000
f+d = 0.01000
f-d = 0.01000
f*d = 0.00000
f/d = 999999977648258.12500
d/f = 0.00000
```

Equality testing

Testing for equality

Never ever ever ever test for equality with floating point numbers!

- Because of rounding errors in floating point numbers, you don't know exactly what you're going to get.
- Instead, test to see if the *absolute difference* is below some *tolerance* that is near epsilon.
- Testing for equality with integers is ok, however, because integers are exact.

```
$ g++ -std=c++17 fp_tol.cpp
$ ./a.out
f*f = 0.01
g = 0.01
False
True
```

```
#include <iostream>
#include <cmath>

int main()
{
    float f = 0.1;
    float g = 0.01;

    std::cout << "f*f = " << f*f << '\n'
              << "g = " << g << '\n';

    if (f*f == g)
        std::cout << "True" << '\n';
    else
        std::cout << "False" << '\n';

    float TOL=1e-7;
    if (fabs(f*f - g) < TOL)
        std::cout << "True" << '\n';
    else
        std::cout << "False" << '\n';
}
```

Roundoff errors

Roundoff error occurs when you're not being careful with which combinations of types of numbers you are operating on:

$$(a + b) + c \neq a + (b + c)$$

```
// RoundOff.cpp

int main()
{
    double a = 1.0, b = 1.0, c = 1e-16;

    std::cout << (a - b) + c << std::endl;
    std::cout << a + (-b + c) << std::endl;
    return 0;
}
```

```
$ g++ -std=c++17 RoundOff.cpp
$ ./a.out
1e-16
1.11022e-16
```

Roundoff errors, continued

Roundoff errors can occur anytime you start operating near machine precision.

- *Machine precision* (or *machine epsilon*) is the upper bound on the relative error due to rounding. This is generally $\approx$ 1e-8 for single precision (float)
  and 1e-16 for double precision.
- Roundoff errors are most common when subtracting or dividing two non-integer numbers that are about the same size, thus forcing the computer to do arithmetic near machine epsilon.
- Do your best to modify your algorithms to avoid such calculations.

Machine epsilon

Machine epsilon

Let's do some addition, to demonstrate what could go wrong.

- Problem: $1.0 + 0.001$
- Let's work in base 10.
- Let's assume that we only have a mantissa precision of 3, and exponent precision of 2.

$$
\begin{array}{r}
1.00 \times 10^{0} \\
+\,1.00 \times 10^{-3} \\
\hline
1.00 \times 10^{0} \\
+\,0.001 \times 10^{0} \\
\hline
1.00 \times 10^{0}
\end{array}
$$

- So what happened?
- Mantissa only has a precision of 3! The final answer is beyond the range of the mantissa!

Machine epsilon

- Machine *epsilon* gives you the limits of the *precision* of the machine.
- It is defined to be the smallest x such that $1 + x \neq 1$.
  (or sometimes, the largest x such that $1 + x = 1$.)
- *Machine epsilon* is named after the mathematical term for a small positive infinitesimal.

```cpp
#include <iostream>
#include <cmath>

int main()
{
  float f = 1.0;
  float g = 1.e-18;

  std::cout << "f =" << f << '\n';
  std::cout << "g =" << g << '\n';

  std::cout << " (1. - 1.)+ 1.e-18 = " << (f-f)+g << '\n';
  std::cout << " (1. + 1.e-18) - 1.0 = " << (f+g)-f << '\n';
  std::cout << " (1. + 1.e-18)  = " << (f+g) << '\n';
}
```

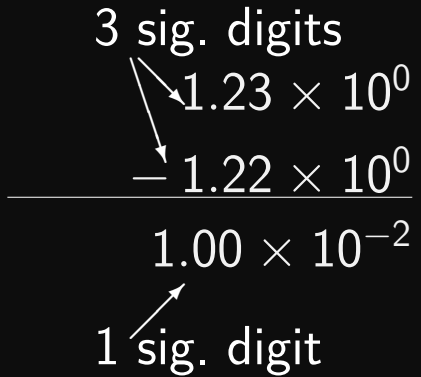
```
$ g++ -std=c++17 fp_machEpsilon.cpp
$ ./a.out
f =10
g =1e-18
(1. - 1.)+ 1.e-18 = 1e-18
(1. + 1.e-18) - 1.0 = 0
(1. + 1.e-18)  = 1
```

Beware: subtraction

Be very wary of subtracting very similar numbers.

- Problem: subtract 1.22 from 1.23.
- Assume that we only have a mantissa precision of 3, and exponent precision of 2.
- By performing this subtraction, we eliminate most of the information, and end up with '*catastrophic cancellation*'.
- We go from 3 significant digits to 1.
- Dangerous in intermediate results.

The same problem can occur when dividing large numbers.



Overflow

Overflow occurs when the result of a calculation exceeds the representable range of the variable type.

- It can happen with different types of numerical types: real (FP), integers, ...
- E.g. 8-bit integers have a range of -128 to 127.
- E.g. 4-bytes floats have a range of $\pm 1.18 \times 10^{-38}$ to $\pm 3.4 \times 10^{+38}$.
- Always be sure to use variables that are big enough for what you're doing.

```cpp
#include <iostream>

int main()
{
  float f = 1.0e15;

  std::cout << "f =" << f << '\n';
  std::cout << "f*f =" << f*f << '\n';
  std::cout << "f*f*f =" << f*f*f << '\n';

}
```

```
$ g++ -std=c++17 fp_machEpsilon.cpp
$ ./a.out
f =1e+15
f*f =1e+30
f*f*f =inf
```

Underflow

An *underflow* error is the opposite of an overflow error: you are attempting to make a number which is smaller than the variable can hold.

- 32-bit floats integers have a range of -3.4e38 to +3.4e38: $(\pm 1.18 \times 10^{-38}, \pm 3.4 \times 10^{+38}]$
- An overflow error will result if you attempt to go beyond this range.
- An underflow error results if you try to go too small.

```cpp
#include <iostream>

int main()
{
  float f = -1.0e35;
  float g = -1.0e44;
  float h = 1.0e40;
  float k = 1.0e-44;
  float l = 1.0e-46;

  std::cout << "f =" << f << '\n';
  std::cout << "g =" << g << '\n';
  std::cout << "h =" << h << '\n';
  std::cout << "k =" << k << '\n';
  std::cout << "l =" << l << '\n';
}
```

```
$ g++ -std=c++17  fp_undFlow.cpp
$ ./a.out
f =-1e+35
g =-inf
h =inf
k =9.80909e-45
l =0
```

Precision is finite $\longrightarrow$ Curb your expectations

- Many numerical algorithms are iterative, and should run until convergence.
- But **you** set at what precision you consider convergence to have occured.

Do no try to converge until machine precision

- Wasteful
- Machine precision is where round of occurs: not meaningful.
- Due to round off, results of seemingly the same computation can differ, or depend on the level of optimization.

Example

```
#include <iostream>
#include <iomanip>
#include <cmath>
/// Compute square root of x by Newton's method
double mysqrt(double x, double relative_tolerance) {
  double sqrtx1 = 0;
  double sqrtx2 = x/2.0;
  //  iterate until solution is close enough
  while (fabs(sqrtx1/sqrtx2 - 1.0)
         >= relative_tolerance) {
     sqrtx1 = sqrtx2;
     sqrtx2 = (sqrtx1+x/sqrtx1)/2;
  }
  return sqrtx2;
}
/// Compute sqrt 20 as an example
int main() {
  std::cout << "sqrt(20)=" << std::setprecision(14)
            << mysqrt(20,1e-4) << " or "
            << sqrt(20) << "\n";
}
```