Numeric Programming Examples

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`http://feynarts.de/lectures/num.pdf`

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Topics

- Mixing Fortran and C
- MathLink Programming
- Floating-point issues
- Alignment and Caching
- “Find the Mistake” Quiz

Mixing Fortran and C

Why Fortran? Why C/C++?

- Around for longer than many modern languages:
  Fortran 1957, C 1972
  Perl 1987, Python 1991, Java 1995, Ruby 1995
- Both widely used, e.g. C in the Linux Kernel.
- Good and free compilers available.
- Being the language of Unix, C is usually the lowest common denominator, i.e. has fewest linking issues.
- Object orientation through Fortran 90/2003, C++. (Introduces name mangling issues, though.)

Mixing Fortran and C

- Most Fortran compilers add an underscore to all symbols.
- Fortran passes all arguments by reference.
- Avoid calling functions (use subroutines) as handling of the return value is compiler dependent.
- ‘Strings’ are character arrays in Fortran and not null-terminated. For every character array the length is passed as an invisible int at the end of the argument list.
- Common blocks correspond to global structs, e.g.

```
double precision a, b
common /abc/ a, b
```

$\leftrightarrow$

```
struct {
  double a, b;
} abc_;
```

- Fortran’s (and C99’s) `double complex` maps onto `struct { double re, im; }`.

MathLink programming

MathLink is Mathematica's API to interface with C and C++.
J/Link offers similar functionality for Java.

A MathLink program consists of three parts:

a) Declaration Section

```
:Begin:
:Function: a0
:Pattern: A0[m_, opt___Rule]
:Arguments: {N[m], N[Delta /. {opt} /. Options[A0]],
   N[Mudim /. {opt} /. Options[A0]]}
:ArgumentTypes: {Real, Real, Real}
:ReturnType: Real
:End:

:Evaluate: Options[A0] = {Delta -> 0, Mudim -> 1}
```

MathLink programming

b) C code implementing the exported functions

```
#include "mathlink.h"

static double a0(const double m,
    const double delta, const double mudim) {
  return m*(1 - log(m/mudim) + delta);
}
```

MathLink programming

c) Boilerplate main function

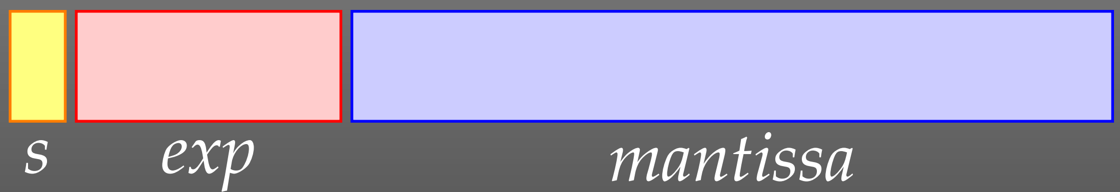
```
int main(int argc, char **argv) {
  return MLMain(argc, argv);
}
```

Compile with `mcc` **instead of** `cc`.
Load in Mathematica with `Install["program"]`.

For even more details see arXiv:1107.4379.

Floating-point Representation

Floating-point numbers are these days always represented internally according to IEEE 754:



- s = sign bit,
- exp = (biased) exponent,
- $mantissa$ = (normalized) mantissa, i.e. implicit MSB = 1.

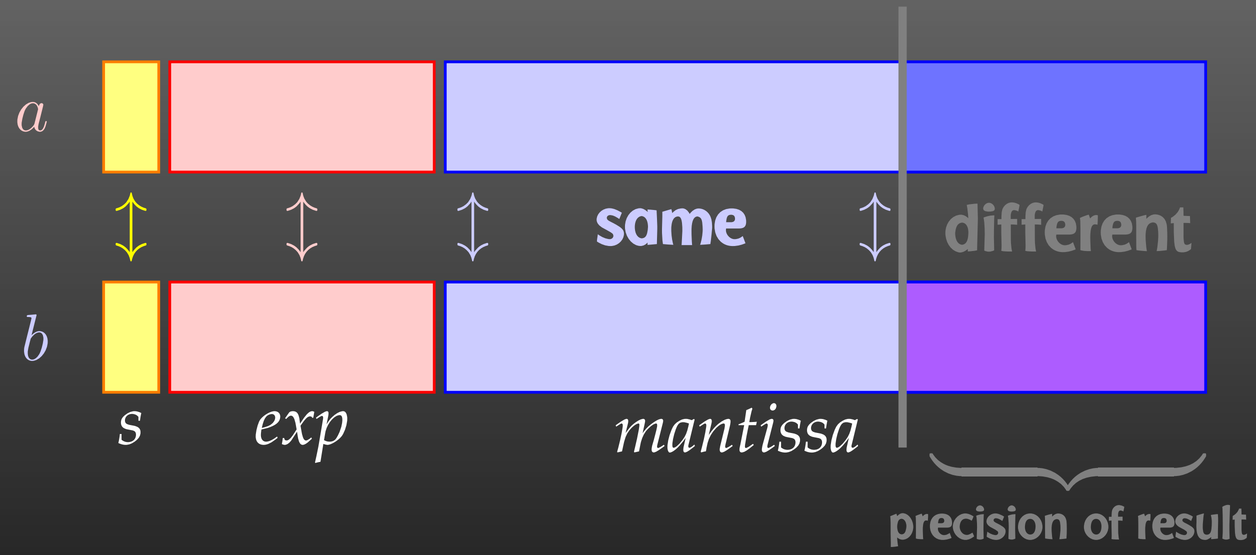
Special values	exponent	mantissa
Zero	0	0
Denormalized numbers	0	non-zero
Infinities	max	0
NaNs	max	non-zero

Bits	exponent	mantissa
Single precision	8	23
Double precision	11	52

Primitive Numerical Optimizations

About the only operation that can seriously cost precision in floating-point arithmetic is subtraction of two similar numbers,

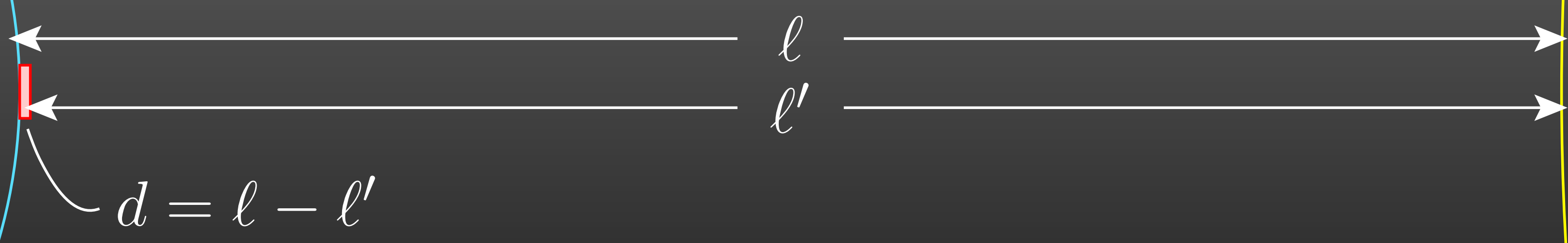
$$a - b, \qquad |a - b| \ll |a| + |b|\,.$$



Floating-point Limits

IEEE 754 codifies the collected experience with many floating-point implementations over several decades.

Double precision is sufficient to measure the thickness d of a pencil to two digits by subtracting the distance ℓ' = earth+pencil–sun from the distance ℓ = earth–sun:



Primitive Numerical Optimizations

Numerical example for loss of precision:

$$\Delta p = p_0 - |\vec{p}| = \sqrt{p^2 + m^2} - p$$

p	m	$\Delta p^{\text{double precision}}$	Δp^{exact}
10^3	1	$.499999875046342 \cdot 10^{-3}$	$.499999875000062 \cdot 10^{-3}$
10^6	1	$.500003807246685 \cdot 10^{-6}$	$.499999999999875 \cdot 10^{-6}$
10^9	1	0	$.500000000000000 \cdot 10^{-9}$
10^{12}	1	0	$.500000000000000 \cdot 10^{-12}$
10^{15}	1	0	$.500000000000000 \cdot 10^{-15}$

Primitive Numerical Optimizations

Always substitute $a^2 - b^2 \to (a-b)(a+b)$.

$a^2 - b^2$ **loses twice as many digits as** $(a-b)(a+b)$**!**

Besides: $a^2 - b^2$ = 2 mul, 1 add, $(a-b)(a+b)$ = 1 mul, 2 add.

Variants on this theme:

- On-shell momentum p:

$$p_0 - p = (p_0 - p)\,\frac{p_0 + p}{p_0 + p} = \frac{m^2}{p_0 + p}$$

- Trigonometry in extreme forward/backward direction:

$$1 - \cos x = (1 - \cos x)\,\frac{1 + \cos x}{1 + \cos x} = \frac{\sin^2 x}{1 + \cos x}$$

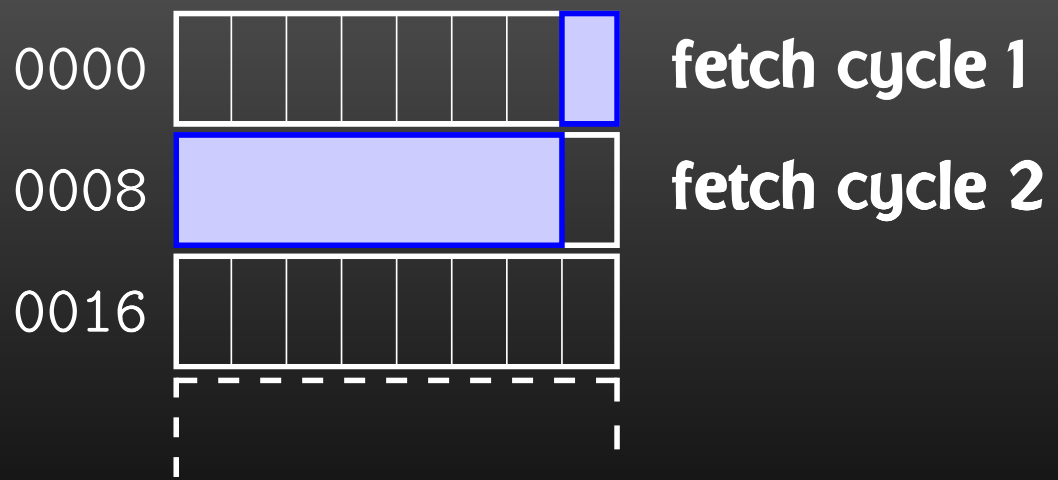
- Polarization vectors:

$$1 - e_z = (1 - e_z)\,\frac{1 + e_z}{1 + e_z} = \frac{e_x^2 + e_y^2}{1 + e_z}$$

Alignment

The CPU generally accesses memory in units of its data bus width, i.e. 4 bytes at a time on a 32-bit machine, 8 bytes at a times on a 64-bit machine.

If a variable is improperly aligned in memory, the CPU needs an extra fetch cycle to read the item! This significantly degrades performance.

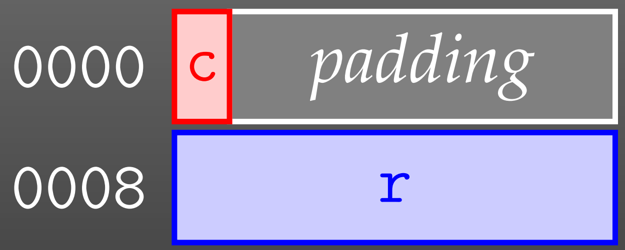


Alignment

Compilers generally align ‘loose’ variables on proper boundaries. Similarly, functions like `malloc` return memory addresses properly aligned for any type of data.

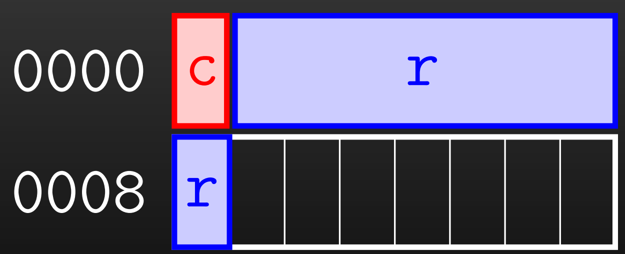
Some languages (e.g. C) allow padding inside structures:

```
struct test {
  char c;
  double r;  };
```



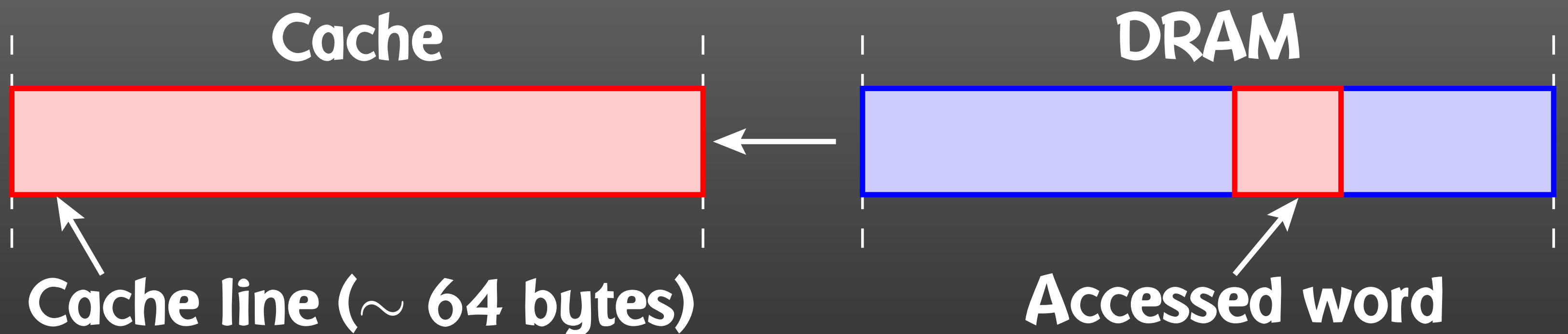
Some languages (e.g. Fortran) do not allow padding, thus the programmer can construct misaligned variables:

```
character*1 c
double precision r
common /test/ c, r
```



Cache

RAM (Random-Access Memory) is in fact not accessed randomly. Modern CPUs have **two levels of cache** 'on top' of the regular RAM. Cache is much faster than DRAM, $t_{\text{cache}} : t_{\text{DRAM}} \approx t_{\text{DRAM}} : t_{\text{disk}}$.



Accessing memory sequentially is typically (much) faster than "hopping around."

Matrix Storage

Due to the cache, accessing a matrix is not arbitrary.

- **Fortran: column-major storage,**
  Matrix = array of column vectors:
  $A_{11} \to A_{21} \to A_{31} \to \ldots$ (first index runs fastest)
- **C: row-major storage,**
  Matrix = array of row vectors:
  $A_{11} \to A_{12} \to A_{13} \to \ldots$ (last index runs fastest)

Naive:

```
do i = 1, n
  do j = 1, n
    sum = sum + A(i,j)
  enddo
enddo
```

Better:

```
do j = 1, n
  do i = 1, n
    sum = sum + A(i,j)
  enddo
enddo
```

Parallelization

In HEP we are (typically) blessed with highly parallelizable problems. For example, computing a cross-section for different point in phase or parameter space.

Such computations are "embarrassingly parallel" – each point can be calculated independently.

How to distribute the iterations automatically without rewriting your program?

Solution: Introduce a serial number

Unraveling Serial Programs

```
     subroutine Computation( range )
     integer serial
     serial = 0
     parameter loop
        ⋮
       serial = serial + 1
       if( serial ∉ range ) goto 1
       (do the computation)
1    enddo
     end
```

Make *range* $\stackrel{\text{e.g.}}{=} i, N$ **accessible from the command line** (`getarg`) **or environment variable** (`getenv`).

Distribution on N machines is now simple:

- **Send serial numbers $1, N+1, 2N+1, \ldots$ to machine 1,**
- **Send serial numbers $2, N+2, 2N+2, \ldots$ to machine 2, etc.**

Simple Parallelization

Simple parallelization using only OS functions can be done using `fork` and `wait`.

`fork` starts new process, returns 0 to child, child-pid to parent.

Unlike `pthread_create`, `fork` creates a completely independent process image. Works even in Fortran.

Linux uses copy-on-write, i.e. memory pages are kept common until either parent or child writes on them.

No simple way to communicate back results to parent.

Find the Mistake

Can you spot what is wrong, undesirable, or potentially dangerous with the following code snippet?

```
inline double KineticEnergy(const double m,
                            const double v) {
  return 1/2*m*v*v;
}
```

Find the Mistake

Can you spot what is wrong, undesirable, or potentially dangerous with the following code snippet?

```
program my_huge_program
double precision radius
print *, "Please enter the radius:"
read(*,*) radius
radius = radius*2*pi
...
```

Find the Mistake

Can you spot what is wrong, undesirable, or potentially dangerous with the following code snippet?

```
subroutine foo(i)
integer i
i = 2*i + 1
end

...

call foo(4711)
```

Find the Mistake

Can you spot what is wrong, undesirable, or potentially dangerous with the following code snippet?

```
#define map(a) 1-a
#define scale(x) 3*x+1

scaled_x = map(scale(x))
```

Find the Mistake

Can you spot what is wrong, undesirable, or potentially dangerous with the following code snippet?

```
block data my_data_ini
double precision half, quarter
common /constants/ half, quarter
data half /1/2D0/
data quarter /1/4D0/
end
```

Find the Mistake

Can you spot what is wrong, undesirable, or potentially dangerous with the following code snippet?

```
double precision x
character*1 id
double complex phase
common /mydata/ x, id, phase
```

Find the Mistake

Can you spot what is wrong, undesirable, or potentially dangerous with the following code snippet?

```
subroutine foo(x)
double precision x
print *, x
end

...

call foo(7.2)
```

Find the Mistake

Can you spot what is wrong, undesirable, or potentially dangerous with the following code snippet?

```
program compute_sum
double precision x(5), sum
integer i
data x /1D40, 4.71D0, -2.5D40, 200D-2, 1.5D40/

sum = 0
do i = 1, 5
  sum = sum + x(i)
enddo
print *, sum
end
```

Exercise

Find an implementation of an extended-precision data type for real numbers using two double-precision numbers, as in:

high part (`real*8`)	low part (`real*8`)

(This is of course not quite the same as quadruple precision.)

Task: program the addition and multiplication operations for such a kind of extended-precision number. The output of each operation should be normalized in the sense that the high part represents the full result to the extent of double precision, e.g. $(10, 10)$ becomes $(20, 0)$ when normalized.

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