

# Numeric Programming Examples

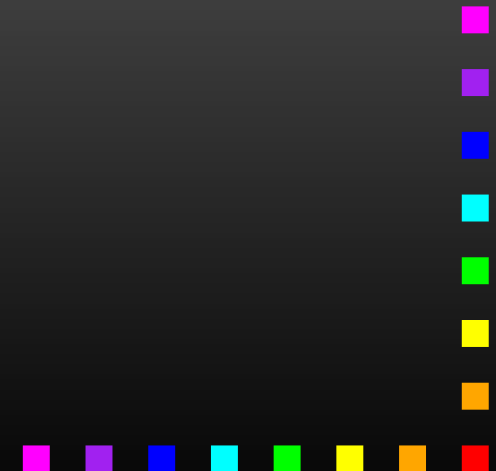
Thomas Hahn

Max-Planck-Institut für Physik  
München



# Some Reference Books

- W.H. Press et al.  
**Numerical Recipes**
- D. Knuth  
**The Art of Computer Programming, 3 Vol.**
- F.S. Acton  
**Real Computing made Real**
- F.S. Acton  
**Numerical Methods that Work**
- C. Dowd, K. Severance  
**High Performance Computing**



# 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      ↔      struct {
common /abc/ a, b        double a, b;
                          } abc_;
```

- **Fortran’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}
```

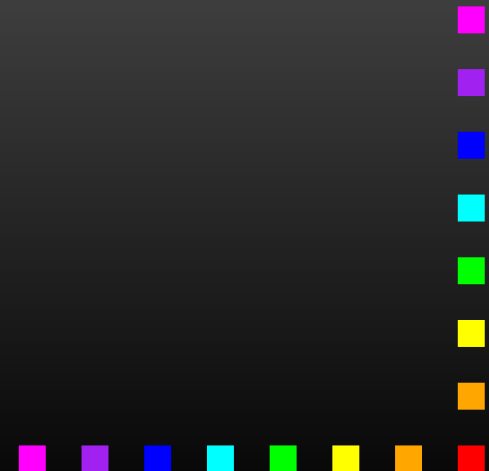


# MathLink programming

## 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);
}
```



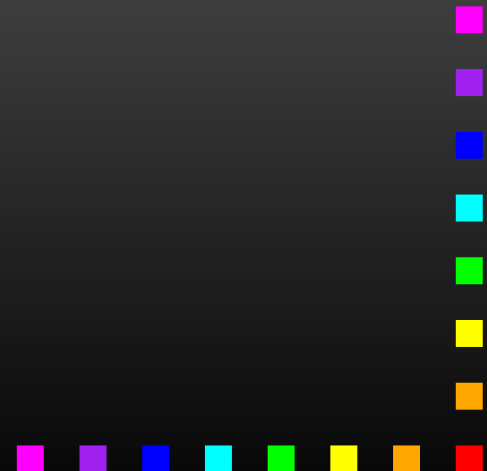
# MathLink programming

## c) Boilerplate main function

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

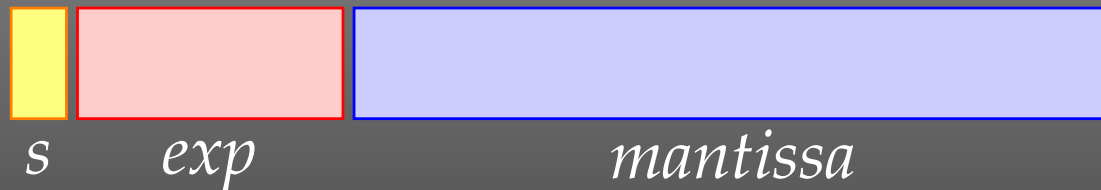
**Compile with `mcc` instead of `cc`.**

**Load in Mathematica with `Install["program"]`.**



# 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.

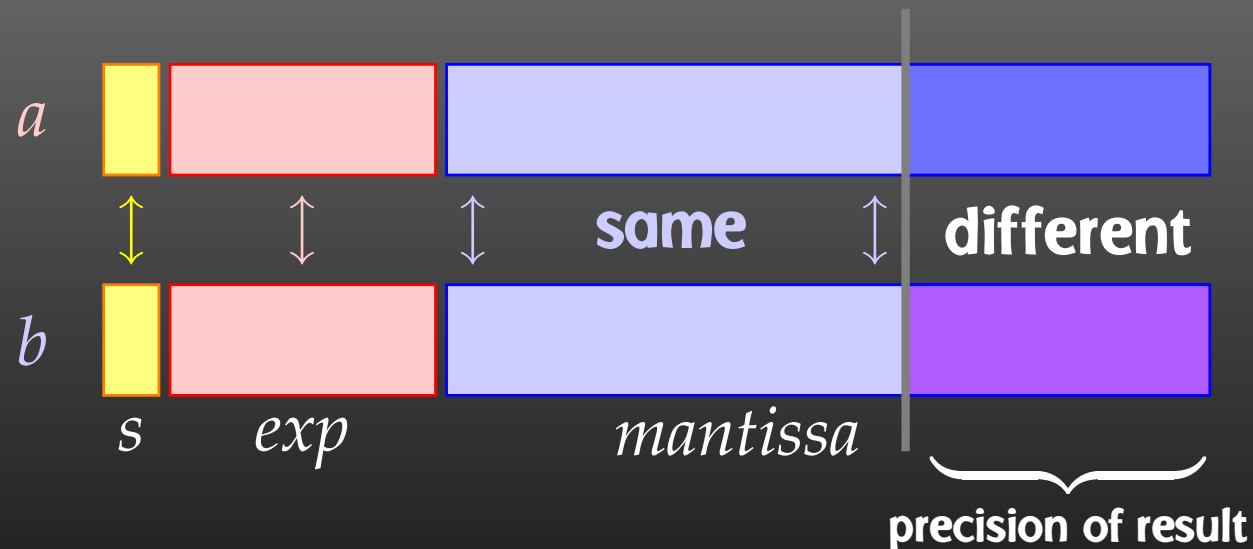
Special values	exponent	mantissa
Zero	0	0
Denormalized numbers	0	non-zero
Infinities	max	0
NaNs	max	non-zero

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**,

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



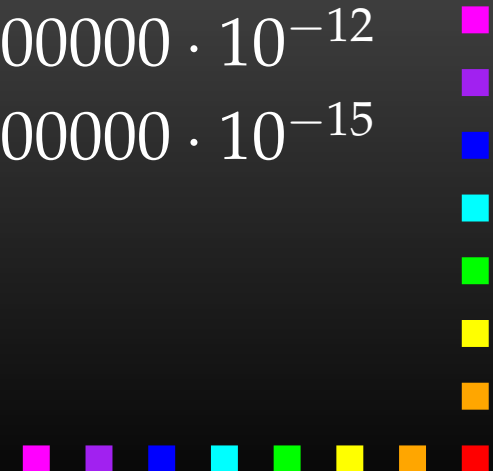


# Primitive Numerical Optimizations

Numerical example for loss of precision:

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

$p$	$m$	$\Delta p^{\text{double precision}}$	$\Delta p^{\text{exact}}$
$10^3$	1	$.4999999875046342 \cdot 10^{-3}$	$.4999999875000062 \cdot 10^{-3}$
$10^6$	1	$.500003807246685 \cdot 10^{-6}$	$.4999999999999875 \cdot 10^{-6}$
$10^9$	1	0	$.5000000000000000 \cdot 10^{-9}$
$10^{12}$	1	0	$.5000000000000000 \cdot 10^{-12}$
$10^{15}$	1	0	$.5000000000000000 \cdot 10^{-15}$



# Primitive Numerical Optimizations

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

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

**Besides:**  $a^2 - b^2 = 2 \text{ mul}, 1 \text{ add}$ ,  $(a - b)(a + b) = 1 \text{ mul}, 2 \text{ add}$ .

**Variants on this theme:**

- **On-shell momentum  $p$ :**

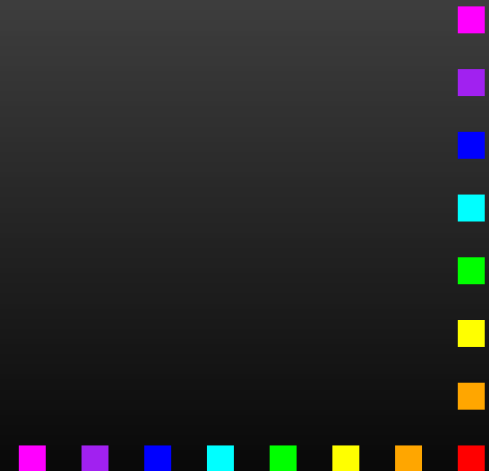
$$p_0 - p = (p_0 - p) \frac{p_0 + p}{p_0 + p} = \frac{m^2}{p_0 + p}$$

- **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:**

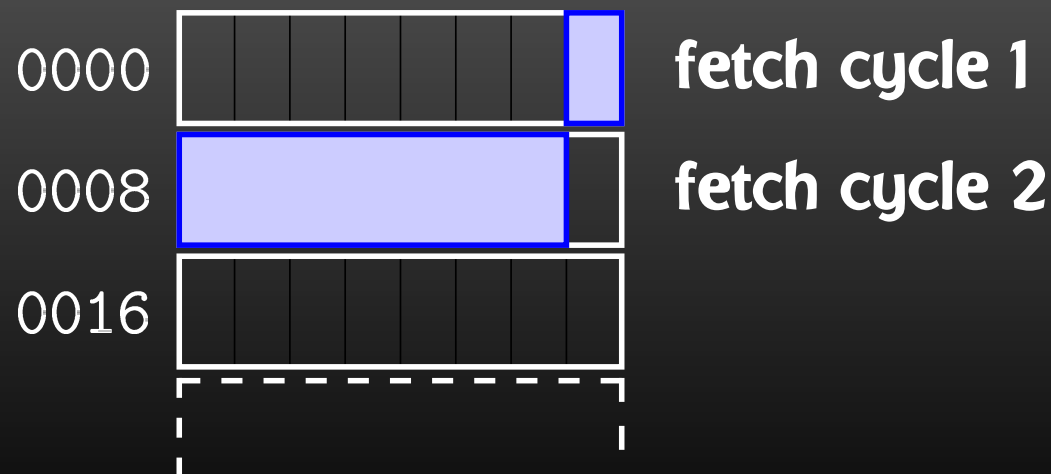
$$1 - e_z = (1 - e_z) \frac{1 + e_z}{1 + e_z} = \frac{e_x^2 + e_y^2}{1 + e_z}$$



# 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 time 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.

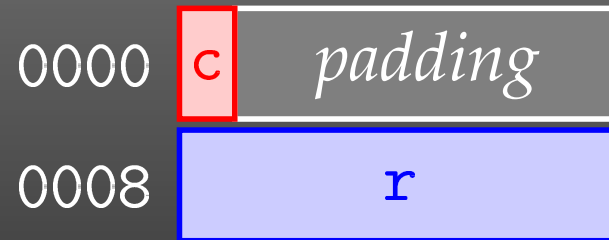


# Alignment

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

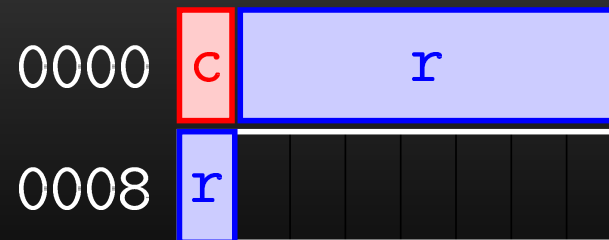
Some languages (e.g. C) **allow padding inside structures:**

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



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

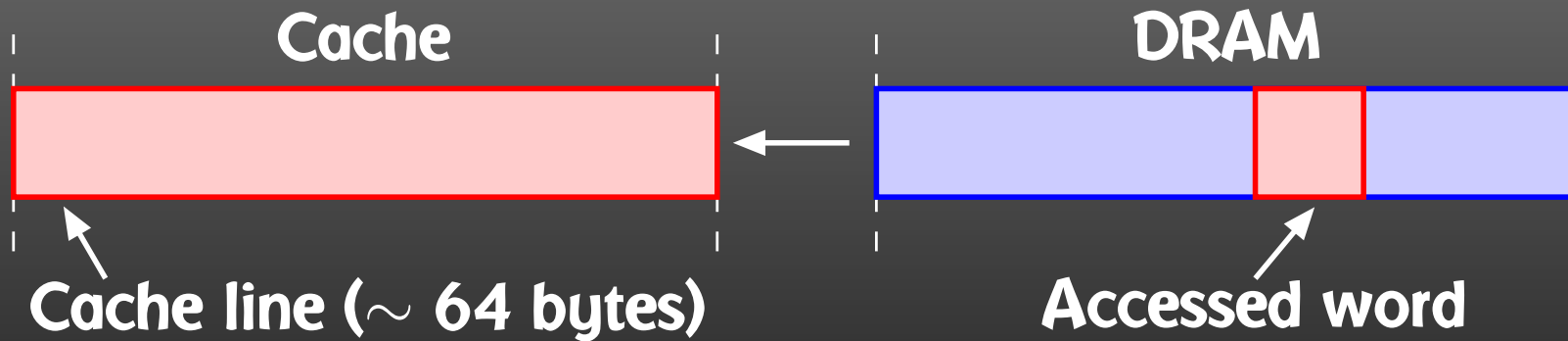
```
character*1 c  
double precision r  
common /test/ c, r
```



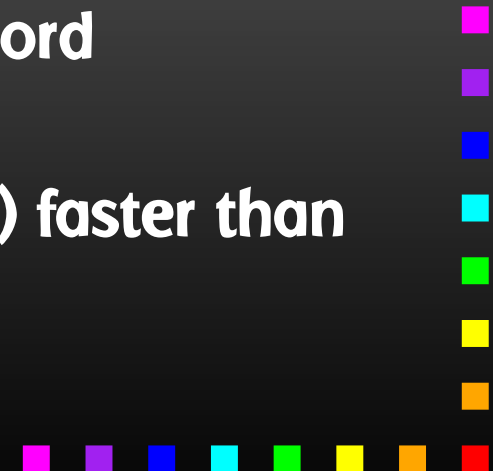
# Cache

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:  
 $A_{11} \rightarrow A_{21} \rightarrow A_{31} \rightarrow \dots$  (first index runs fastest)
- **C: row-major storage,**  
Matrix = array of row vectors:  
 $A_{11} \rightarrow A_{12} \rightarrow A_{13} \rightarrow \dots$  (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
```



## Quiz

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;  
}
```



## Quiz

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
...
```





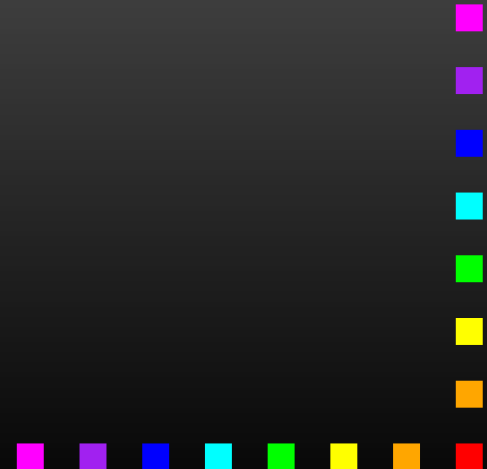
# Quiz

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)
```



## Quiz

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))
```



## Quiz

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
```



# Quiz

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
```



# Quiz

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)
```



## Quiz

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
```

