Vincenzo Innocente:

"Optimal floating point computation"

Accuracy, Precision, Speed in scientific computing

- IEEE 754 standard
- Expression optimization
- Approximate Math

- X86_64 SIMD instructions
- Vectorization using the GCC compiler

Objectives

- Understand precision and accuracy in floating point calculations
- Manage optimization, trading precision for speed (or vice-versa!)
- Understand and Exploit vectorization
- Learn how to make the compiler to work for us

Prepare for the excercises

cd hands-on

cd floatingpoint

c++ –O2 –Wall –march=native floats.cpp

./a.out

Try

https://gcc.godbolt.org/

Disclaimer, caveats, references

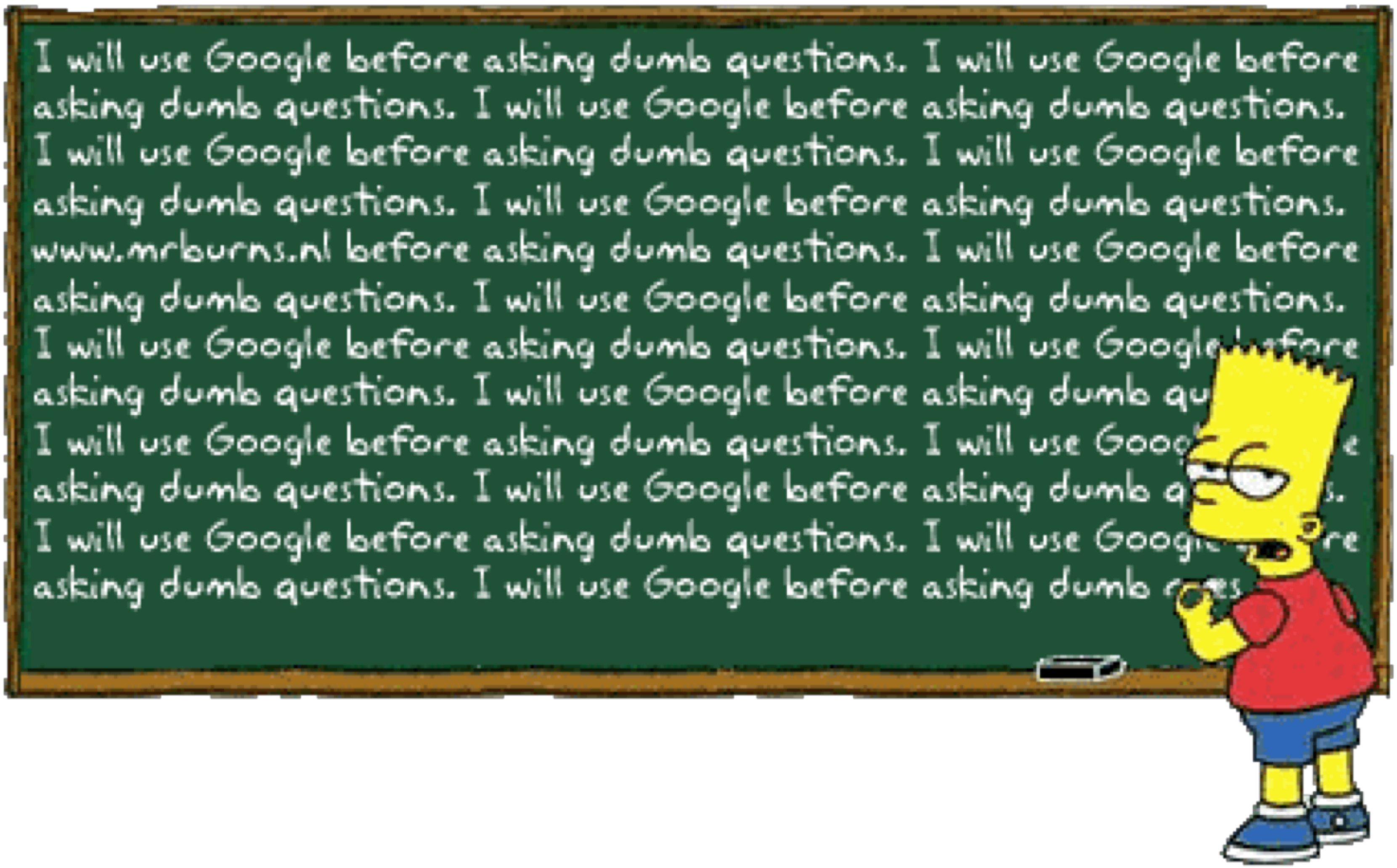
- This is NOT a full overview of IEEE 754
- It applies to x86_64 systems and gcc > 4.7.0
  - Other compilers have similar behavior, details differ
- General References
  - Wikipedia has excellent documentation on the IEEE 754, math algorithms and their computational implementations
  - Handbook of Floating-Point Arithmetic (as google book)
  - Kahan home page
  - INTEL doc and white papers (including ColFax web site)
  - MetaLibm site

Applicability

- It is very (very) different if you deal with
  - Video games
  - Analysis of scientific data
  - Financial applications (with legal bindings)
  - Real time applications
  - Human-life

- http://www.heidelberg-laureate-forum.org/blog/video/lecture-thursday-september-26-william-morton-kahan/

Don’t be afraid to ask questions!

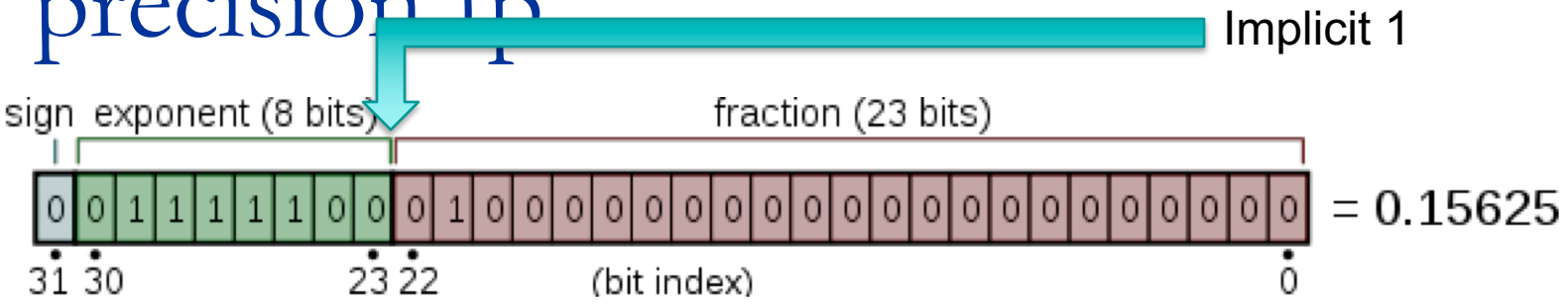


Floating Point Representation

(source Wikipedia)

- floating point describes a system for representing numbers that would be too large or too small to be represented as integers.
  - The advantage of floating-point representation over fixed-point (and integer) representation is that it can support a much wider range of values.
    - int: −2,147,483,648 to +2,147,483,647, $-(2^{31})\sim(2^{31}-1)$
    - float: 1.4×10^{-45} to 3.4×10^{38}
    - double: $\sim 10^{-323}$ to $\sim 10^{308}$
  - This has a cost…

IEEE 754 representation of single precision fp



$$n = (-1)^s \times (m2^{-23}) \times 2^{x-127}$$

Exponent	significand zero	significand non-zero	Equation
00_H	zero, −0	subnormal numbers	$(-1)^{signbits} \times 2^{-126} \times$ 0.significandbits
01_H, ..., FE_H	normalized value	normalized value	$(-1^{signbits} \times 2^{exponentbits-127} \times$ 1.significandbits
FF_H	±infinity	NaN (quiet,signalling)	

Floating Point Types

Type	Sign	Exponent	Significand field	Total bits	Exponent bias	Bits precision	Number of decimal digits
Half (IEEE 754-2008)	1	5	10	16	15	11	~3.3
Single	1	8	23	32	127	24	~7.2
Double	1	11	52	64	1023	53	~15.9
x86 extended precision	1	15	64	80	16383	64	~19.2
Quad	1	15	112	128	16383	113	~34.0

- Half : __fp16, available for storage on recent ARM, INTEL and NVIDIA HW
- Single: float, storage and computation in C++ on any hardware
- Double: double, storage and computation in C++ on any hardware
- Ext-precision: long double, No storage! computation in C++ on x86 hardware
- Quad: __float128, storage and (software) computation in C++

C++ interlude

```
#include<iostream>
#include<iomanip>
#include<cmath>
#include<limits>
//  std style
template<typename T>
void print(T x) {
 std::cout << std::hexfloat << x <<' ' // exact binary representation
           <<  std::scientific << std::setprecision(8) << x << ' ' // 8 decimal digits
           <<  std::defaultfloat << x << std::endl;    // 6 decimal digits for float
}

// integer representation
#include<cstring>
#include<bitset>
int f2i(float x) { int i; memcpy(&i,&x,sizeof(int)); return i;} // compiler will optimize
//  use bitset to print in binary (bit by bit)
std::cout << std::bitset<32>(f2i(x)) << std::endl; ;   // bit by bit
```

Limits

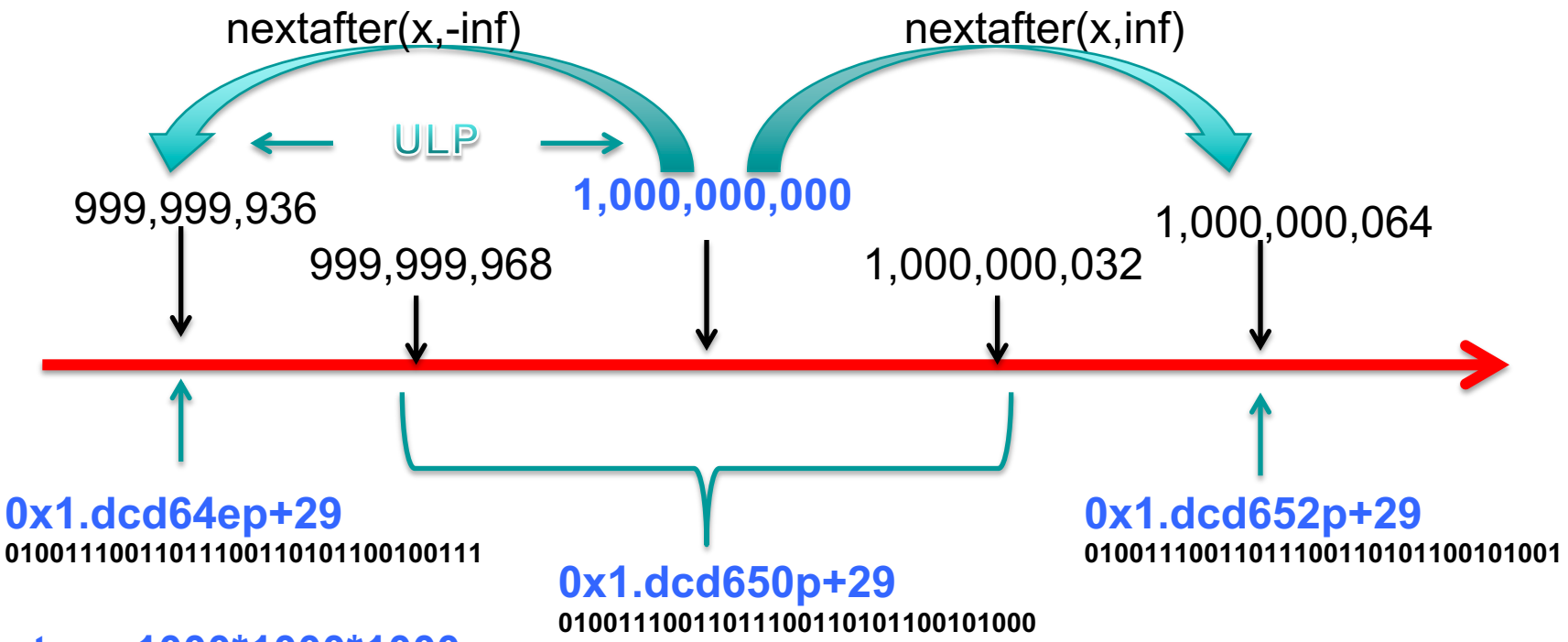
- Everything you want to know about an arithmetic type is in
  - std::numeric_limits<T>
  - see http://www.cplusplus.com/reference/limits/numeric_limits/

```
#include <iostream>     // std::cout
#include <limits>       // std::numeric_limits
int main () {
  std::cout << std::boolalpha;
  std::cout << "Minimum value: " << std::numeric_limits<float>::min() << '\n';
  std::cout << "Maximum value: " << std::numeric_limits<float>::max() << '\n';
  std::cout << "Is signed: " << std::numeric_limits<float>::is_signed << '\n';
  std::cout << "significand bits: " << std::numeric_limits<float>::digits << '\n';
  std::cout << "precision: " << std::numeric_limits<float>::epsilon() << '\n';
  std::cout << "has infinity: " << std::numeric_limits<float>::has_infinity << '\n';
  return 0;
}
```

examples

		sign	exponent	significant
0.00000000e+00	0x0p+0	0	00000000	00000000000000000000000
5.00000000e-01	0x1p-1	0	01111110	00000000000000000000000
1.00000000e+00	0x1p+0	0	01111111	00000000000000000000000
1.50000000e+00	0x1.8p+0	0	01111111	10000000000000000000000
2.00000000e+00	0x1p+1	0	10000000	00000000000000000000000
2.50000000e+00	0x1.4p+1	0	10000000	01000000000000000000000
3.00000000e+00	0x1.8p+1	0	10000000	10000000000000000000000
8.00000000e+00	0x1p+3	0	10000010	00000000000000000000000
3.14159274e+00	0x1.921fb6p+1	0	10000000	10010010000111111011011
1.00000001e-01	0x1.99999ap-4	0	01111011	10011001100110011001101
1.17549435e-38	0x1p-126	0	00000001	00000000000000000000000
3.40282347e+38	0x1.fffffep+127	0	11111110	11111111111111111111111
nan	nan	1	11111111	10000000000000000000000
-inf	-inf	1	11111111	00000000000000000000000
2.93873588e-39	0x1p-128	0	00000000	01000000000000000000000

Precision, rounding



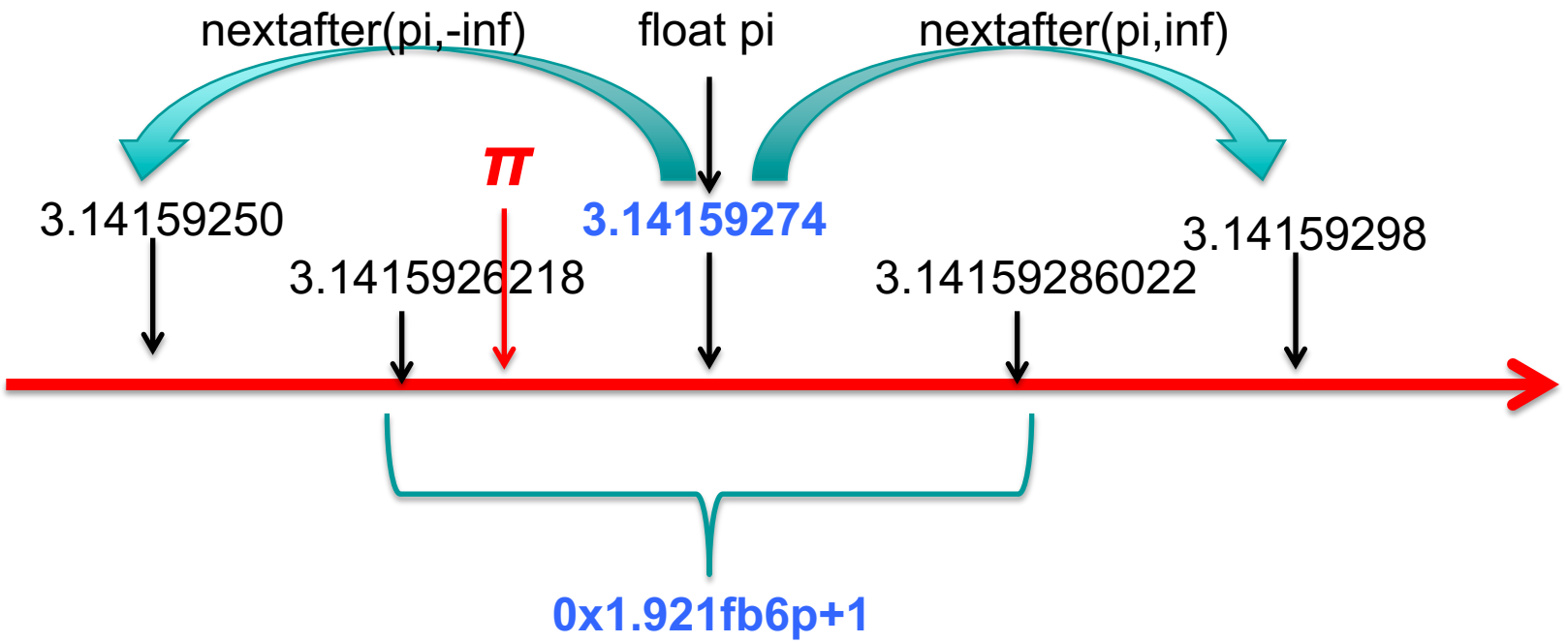
float x = 1000*1000*1000;

```
std::cout <<  std::scientific << std::setprecision(8)
          << x << ' ' << x+32.f << ' ' << x+33.f << std::endl
          << x+32.f-x << x+33.f-x << std::endl;
```

1.00000000e+09 1.00000000e+09 1.00000006e+09
0.00000000e+00 6.40000000e+01

https://en.wikipedia.org/wiki/Unit_in_the_last_place

Precision, rounding



float pi = M_PI; // 0x1.921fb54442d18p+1 3.1415926535897931e+00

Double precision!

Rounding Algorithms

- The standard defines five rounding algorithms.
  - The first two round to a nearest value; the others are called directed roundings:
- Roundings to nearest
  - **Round to nearest, ties to even – rounds to the nearest value;** if the number falls midway it is rounded to the nearest value with an even (zero) least significant bit, which occurs 50% of the time; this is the default algorithm 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)
- 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).

Loss of precision

Summing *many* values

```
float x1=0;
for (float y=1;y<=1000000; ++y) x1+=y;
print (x1); // 4.99941376e+11 4.9994138e+11 0x1.d19b5p+38

float x2=0;
for (float y=1000000;y>0; --y) x2+=y;
print (x2); // 4.99873677e+11 4.9987368e+11 0x1.d18b2cp+38

int N=16; float xx[N];  for (int i=0; i<N; ++i) xx[i]=0;
for (int i=0; i<N; ++i)
for (int y=i;y<=1000000; y+=N) xx[i]+=float(y);
float s=0; for (int i=0; i<N; ++i) s+=xx[i];
print (s); // 4.99999900e+11 4.999999e+11 0x1.d1a944p+38

float result = 0.5*1000000 *(1000000+1);
std::cout << std::scientific << (result-x1)/result << "    "
          << (result-x2)/result << "    " << (result-s)/result << std::endl;
// 1.18226832e-04      2.53624079e-04   1.17964680e-06

float x3=0; float tenth=0.1f;
for(int i=0; i<10000;++i) x3+=tenth;
print(x3); // 9.99902893e+02 999.90289 0x1.f3f392p+9 (google for: patriot failure)
```

Loss of precision

Cancellations: Subtracting *too-close* values

For example, consider the quadratic equation:

$$ax^2 + bx + c = 0,$$

with the two exact solutions:

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$

Better solution

$$x_1 = \frac{-b - \operatorname{sgn}(b)\sqrt{b^2 - 4ac}}{2a},$$

$$x_2 = \frac{2c}{-b - \operatorname{sgn}(b)\sqrt{b^2 - 4ac}} = \frac{c}{ax_1}.$$

Two sources of cancellation

https://en.wikipedia.org/wiki/Loss_of_significance

Loss of precision

To illustrate the instability of the standard quadratic formula *versus* this variant formula, consider a quadratic equation with roots 1.786737589984535 and $1.149782767465722 \times 10^{-8}$. To sixteen significant figures, roughly corresponding to double-precision accuracy on a computer, the monic quadratic equation with these roots may be written as:

$$x^2 - 1.786737601482363x + 2.054360090947453 \times 10^{-8} = 0$$

Using the standard quadratic formula and maintaining sixteen significant figures at each step, the standard quadratic formula yields

$$\begin{aligned}
\sqrt{\Delta} &= 1.786737578486707 \\
x_1 &= (1.786737601482363 + 1.786737578486707)/2 = 1.786737589984535 \\
x_2 &= (1.786737601482363 - 1.786737578486707)/2 = 0.000000011497828
\end{aligned}$$

Note how cancellation has resulted in x_2 being computed to only eight significant digits of accuracy. The variant formula presented here, however, yields the following:

$$\begin{aligned}
x_1 &= (1.786737601482363 + 1.786737578486707)/2 = 1.786737589984535 \\
x_2 &= 2.054360090947453 \times 10^{-8} / 1.786737589984535 = 1.149782767465722 \times 10^{-8}
\end{aligned}$$

Note the retention of all significant digits for x_2.

Floating Point Math

- Floating point numbers are NOT real numbers
  - They exist in a finite number (~2^{32} for single prec)
    - Exercise: count how many floats exists between given two
  - Exist a “next” and a “previous” (std::nextafter)
    - Differ of one ULP (Unit in the Last Place or Unit of Least Precision http://en.wikipedia.org/wiki/Unit_in_the_last_place)
  - Results of Operations are rounded
    - Standard conformance requires half-ULP precision.
    - $x + \varepsilon - x \neq \varepsilon$ (can easily be 0 or ∞)
  - Their algebra is not associative
    - $(a+b) + c \neq a+(b+c)$
    - $a/b \neq a*(1/b)$
    - $(a+b)*(a-b) \neq a^2 - b^2$

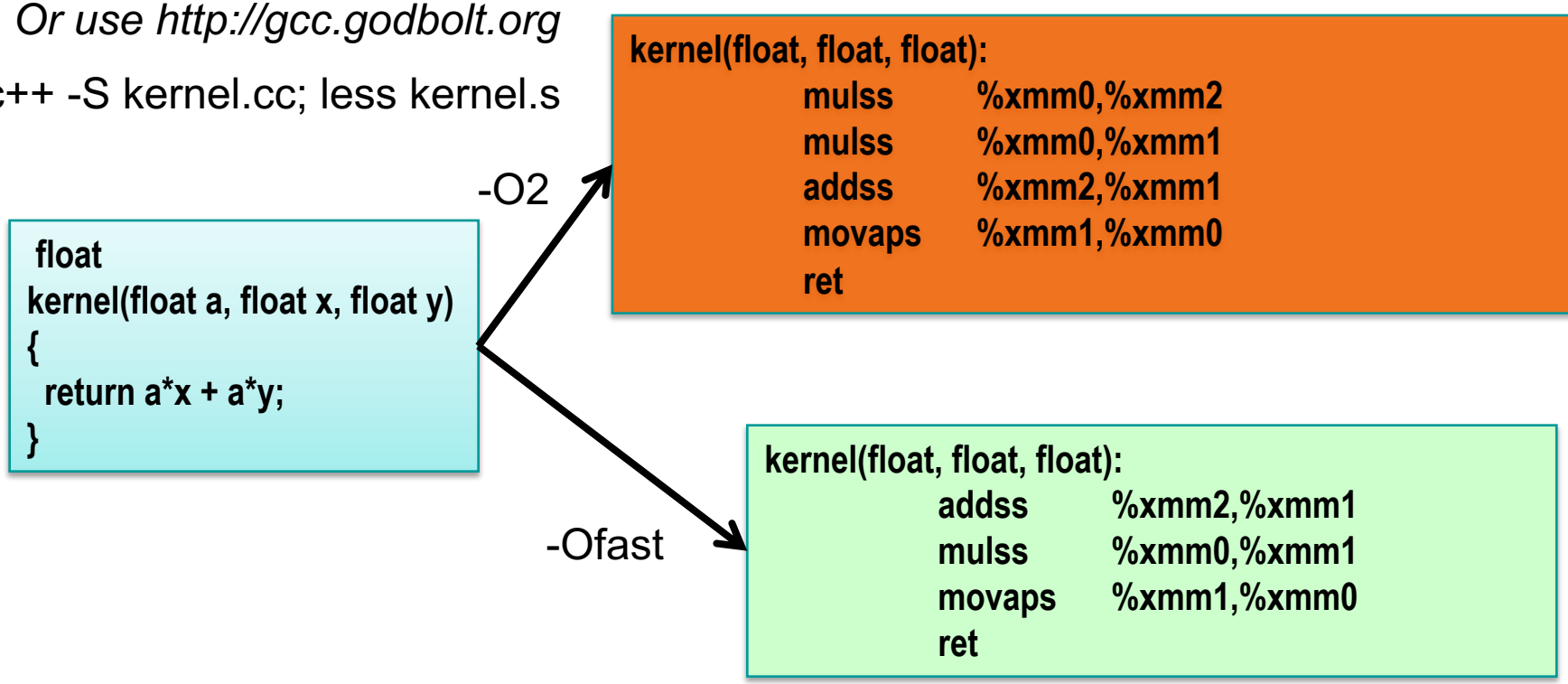
Strict IEEE754 vs "Finite" (fast) Math

- Compilers can treat FP math either in "strict IEEE754 mode" or optimize operations using "algebra rules for finite real numbers" (as in FORTRAN)
  - gcc default is "strict IEEE754 mode"
  - –O2 –funsafe-math –ffast-math
  - –Ofast (switch vectorization on as well)
    - Caveat: the compiler improves continuously: still it does not optimize yet all kind of expressions
- https://gcc.gnu.org/wiki/FloatingPointMath

Inspecting generated code

objdump -S -r -C --no-show-raw-insn –w kernel.o | less
(on MacOS: otool -t -v -V –X kernel.o | c++filt | less)
Or use http://gcc.godbolt.org

c++ -S kernel.cc; less kernel.s



Exercise: compare assembler for O2 and Ofast
http://goo.gl/5jwOVO

FMA (fused multiply add)

- fma(a,b,c) = round(a*b+c)
  - Opposed to round(round(a*b)+c)
- Single instruction with 4 or 5 cycle latency
  - Opposed to 2 instructions with 5+3 cycle latency
- More precise (one rounding instead of two)
  - Results will differ!
- Introduce a “contraction” issue
  - No standard contraction rules (yet)
  - a*b+c*d , a+b*c+d , x*=a;x+=b , etc

Controlling fma (contraction)

- gcc (and clang) flags
  - `-ffp-contract=off` (default is "`fast`")
  - https://stackoverflow.com/questions/43352510/difference-in-gcc-ffp-contract-options
- cuda (nvcc) flags
  - `-fmad=false` (default is "`true`")
  - https://docs.nvidia.com/cuda/floating-point/index.html

fma library function

- std::fma
  - Implemented in software (libm)
    - Used if fma instruction not supported: SLOW
  - Compilers will use fma instruction if exists
    - Not affected by re-association flags
- To fully control fma and be fully reproducible
  - use std::fma
  - disable “contraction”

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^{-38} to 10^{-45}
- Subnormals guarantee that additions never underflow
  - Any other operation producing *a subnormal* will raise a underflow exception if also inexact
- Literature is full of very good reasons why “gradual underflow” improves accuracy
  - This is why they are part of the IEEE 754 standard
- 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* subnormals
  - It will raise underflow and inexact exceptions

Floating point exceptions

The IEEE floating point standard defines several exceptions that occur when the result of a floating point operation is unclear or undesirable. Exceptions can be ignored, in which case some default action is taken, such as returning a special value. When trapping is enabled for an exception, an error is signalled whenever that exception occurs. These are the possible floating point exceptions:

- **Underflow:** This exception occurs when the result of an operation is too small to be represented as a normalized float in its format. If trapping is enabled, the *floating-point-underflow* condition is signalled. Otherwise, the operation results in a denormalized float or zero.
- **Overflow:** This exception occurs when the result of an operation is too large to be represented as a float in its format. If trapping is enabled, the *floating-point-overflow* exception is signalled. Otherwise, the operation results in the appropriate infinity.
- **Divide-by-zero**: This exception occurs when a float is divided by zero. If trapping is enabled, the *divide-by-zero* condition is signalled. Otherwise, the appropriate infinity is returned.
- **Invalid:** This exception occurs when the result of an operation is ill-defined, such as (0.0/ 0.0). If trapping is enabled, the *floating-point-invalid* condition is signalled. Otherwise, a quiet NaN is returned.
- **Inexact:** This exception occurs when the result of a floating point operation is not exact, i.e. the result was rounded. If trapping is enabled, *the floating-point-inexact* condition is signalled. Otherwise, the rounded result is returned.

Defensive Computing

- Verify pre/post conditions and algorithm invariants
- Strict IEEE754 conformance
- In case of invalid input notify
  - Exception
  - Error code
  - Nan, inf..
- Can be implemented as a wrapper of a HPC algo

High Performance

- Garbage in, garbage out
- Assume finite math
- Invalid input
  - Undefined behavior
  - Algorithm processes it at no additional cost
- User responsibility to guarantee correctness

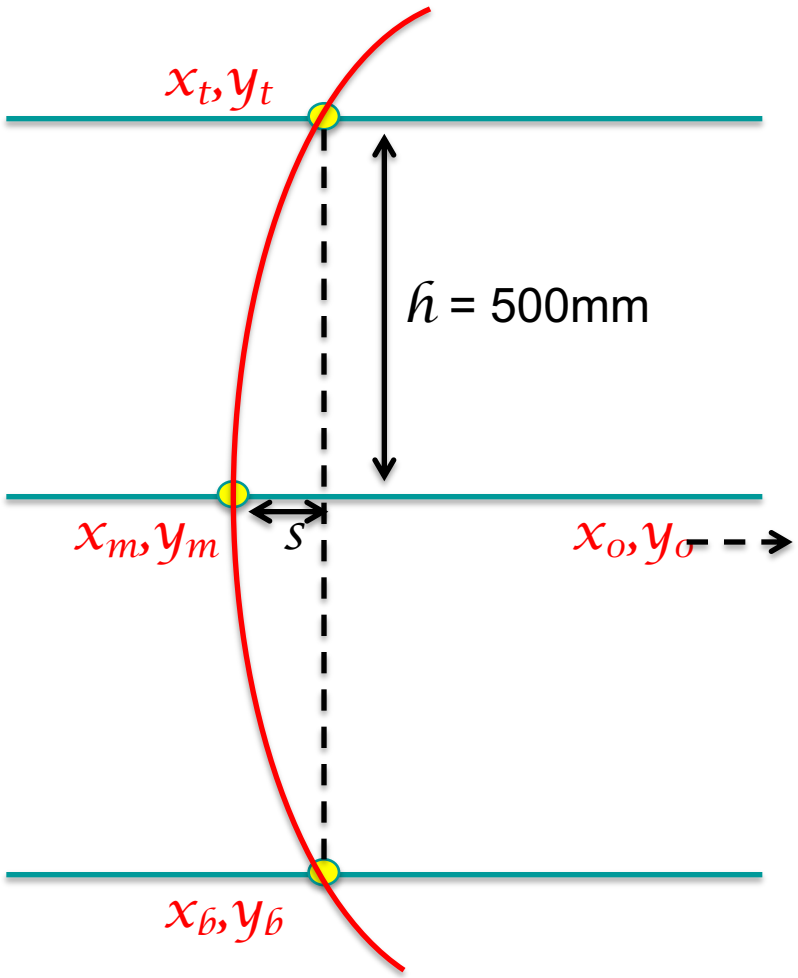
In https://gcc.godbolt.org/z/OmNMxx change -O3 in -Ofast

PRECISION, ACCURACY, SPEED

Definitions (mine)

- Precision
  - Numerical precision (in bits)
  - Can be evaluated using a higher “precision”
- Accuracy
  - The error w/r/t the truth
  - Can be evaluated comparing different algorithms
- Target Accuracy
  - The acceptable tolerance w/r/t the above
  - Evaluated, for instance, w/r/t know error on the truth

Example: detector of size 1 m and resolution 10 micron (required accuracy: ~1micron?)



three measurement planes

Is single precision enough to represent
- geometric elements?
- Measurements?
- computed trajectory?

Is enough to perform computation?

Trajectory: circle with radius r
s is the sagita, h the half-chord

$r = (s^2+h^2)/2s \sim h^2/2s$
$h^2 = 2sr - s^2$
$x_o = r + x_m$

Circle equation and solutions

$(x-x_o)^2 + (y-y_o)^2 = r^2$

Compute x_t (*x for* $y=h$)

$x = x_o - (r^2 - h^2)^{1/2} \sim 0$ (*zero*)

Alternative formulation equivalent to change of coordinate centered at x_m, y_m

$(x-x_m)^2 + (y-y_m)^2 - 2ar(x-x_m) - 2br(y-y_m) = 0$

In our case $a=1$, $b=0$

$(x-x_m)^2 - 2(x-x_m)r + h^2 = 0$

$x = x_m + h^2 / (r + (r^2 - h^2)^{1/2}) \sim x_m + h^2 / 2r$

A correct choice of algorithm can allow to use a reduced precision to obtain the same accuracy

- Faster
- Smaller memory footprint

PRECISION, ACCURACY, SPEED

Cost of operations (in cpu cycles)

op	instruction	sse s	sse d	avx s	avx d (FMA s&d)
+,-	ADD,SUB	3	3	3	3 4
== < >	COMISS CMP..	2,3	2,3	2,3	2,3
f=d d=f	CVT..	3	3	4	4
|,&,^	AND,OR	1	1	1	1
*	MUL	5	5	5	5 4
/,sqrt	DIV, SQRT	10-14	10-22	21-29	21-45
1.f/ , 1.f/sqrt	RCP, RSQRT	5		7	
=	MOV	1,3,…	1,3,…	1,4,….	1,4,… ➔350 from main memory

Approximate reciprocal (sqrt, div)

The major contribution of game industry to SE is the discovery of the “magic” fast 1/√x algorithm

```
float invSqrt(float x){
  int i;  memcpy(&i,&x,4);
  i = 0x5f3759df – (i >> 1);
  float y; memcpy(&y,&i,4);// approximate
  return y * (1.5f - 0.5f * x * y * y); // better
}
```

Compilers use them at Ofast
Accuracy 2ULP
Non standard: Hardware dependent

Real x86_64 code for 1/√x

```
 _mm_store_ss( &y, _mm_rsqrt_ss( _mm_load_ss( &x ) ) );
return y * (1.5f - 0.5f * x * y * y); // One round of Newton's method
```

Real x86_64 code for 1/x

```
_mm_store_ss( &y,_mm_rcp_ss( _mm_load_ss( &x ) ) );
 return (y+y) – x*y*y; // One round of Newton's method
```

Cost of functions (in cpu cycles i7sb)

	Gnu libm (~IEEE754 compliant)		VDT (Cephes) (~1ULP precise)	
	single	double	single	double
sin,cos,tan	55	100	30	50
large x	***>500***			
sincos	70		40	
atan2	50	100	30	45
exp	***650***	65	42	55
log	50	105	37	42

SET_RESTORE_ROUND_NOEXF (FE_TONEAREST);

Precision vs Speed in "libm"

- Log
  - 24 bit precision needs 8th degree polynomial
  - 16 bit precision needs 5th degree polynomial
  - 7 bit precision needs 2th degree polynomial

	2	3	4	5	6	7	8
e^x	6.8	10.8	15.1	19.8	24.6	29.6	34.7
$\sin(x)$	7.8	12.7	16.1	21.6	25.5	31.3	35.7
$\ln(1+x)$	8.2	11.1	14.0	16.8	19.6	22.3	25.0
$\arctan(x)$	8.7	9.8	13.2	15.5	17.2	21.2	22.3
$\tan(x)$	4.8	6.9	8.9	10.9	12.9	14.9	16.9
$\arcsin(x)$	3.4	4.0	4.4	4.7	4.9	5.1	5.3
$\sqrt{x}$	3.9	4.4	4.8	5.2	5.4	5.6	5.8

Number of significant bits of accuracy vs degree of minimax polynomial approximating the range [0..1].

Example: multiple scattering formula

```
double ms(double radLen, double m2, double p2) {
  constexpr double amscon = 1.8496e-4;    // (13.6MeV)**2
  double e2     = p2 + m2;
  double beta2  = p2/e2;
  double fact = 1 + 0.038*log(radLen);  fact *=fact;
  double a = fact/(beta2*p2);
  return amscon*radLen*a;
}
```

Already an approximation

Material density, thickness, track angle
Known at percent?

```
float msf(float radLen, float m2, float p2) {
  constexpr float amscon = 1.8496e-4;    // (13.6MeV)**2
  float e2     = p2 + m2;

  float fact = 1.f + 0.038f*unsafe_logf<2>(radLen); fact /= p2;
  fact *=fact;
  float a = e2*fact;
  return amscon*radLen*a;
}
```

2nd order polynomial

How to speed up math

- Avoid or factorize-out division and sqrt
  - if possible compile with “–Ofast”
- 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

Example: cut in pt, phi, eta

```
inline float pt2(float x, float y) {return x*x+y*y;}
inline float pt(float x, float y) {return std::sqrt(pt2(x,y));}
inline float phi(float x, float y) {return std::atan2(y,x);}
inline eta(float x, float y, float z) { float t(z/pt(x,y)); return ::asinhf(t);}
inline float dot(float x1, float y1, float x2, float y2) {return x1*x2+y1*y2;}
Inline float dphi(float p1,float p2) {
    auto dp=std::abs(p1-p2); if (dp>float(M_PI)) dp-=float(2*M_PI);
    return std::abs(dp);
};
```

```
if (pt(x[i],y[i])>ptcut) …

if (dphi(phi(x[i],y[i]),phi(x[j],y[j]))<phicut) ….
```

Exercise in ptcut.cpp

Formula Translation: what was the author's intention?

```
// Energy loss and variance according to Bethe and Heitler, see also
 // Comp. Phys. Comm. 79 (1994) 157.
 //
 double p = mom.mag();
 double normalisedPath = fabs(p/mom.z())*radLen;
 double z = exp(-normalisedPath);
 double varz = (exp(-normalisedPath*log(3.)/log(2.))- exp(-2*normalisedPath));
```

```
double pt = mom.perp();
double j = a_i*(d_x * mom.x() + d_y * mom.y())/(pt*pt);
double r_x = d_x - 2* mom.x()*(d_x*mom.x()+d_y*mom.y())/(pt*pt);
double r_y = d_y - 2* mom.y()*(d_x*mom.x()+d_y*mom.y())/(pt*pt);
double s = 1/(pt*pt*sqrt(1 - j*j));
```

Exercise: edit OptimizeIt.cc to make it "optimal"
check the generated assembly, verify speed gain

Formula Translation: the solution?

Is the compiler able to do it for us?

SIMD: LOOP VECTORIZATION

Test environment

cd hands-on/vectorization

c++ -O2 pi.cpp -fopt-info-vec -march=native; time ./a.out

c++ -Ofast pi.cpp -fopt-info-vec -march=native; time ./a.out

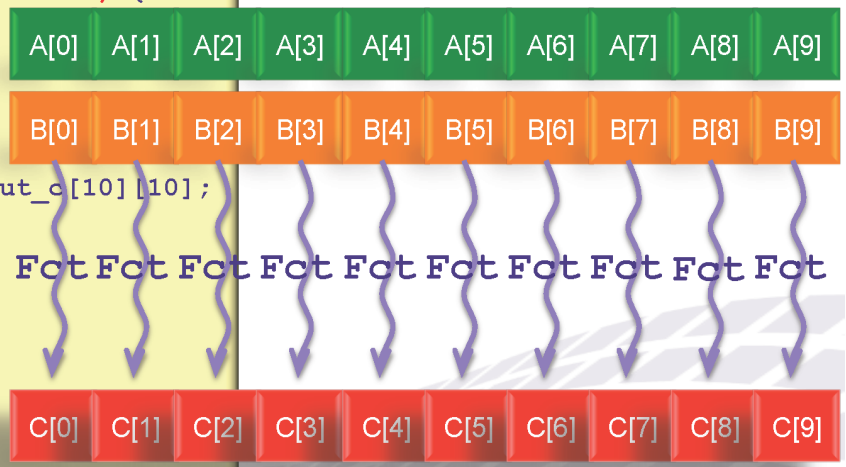
What is Stream Computing?

CAPS

- A similar computation is performed on a collection of data (*stream*)
  - There is no data dependence between the computation on different stream elements
- Stream programming is well suited to GPU *and vector-cpu!*

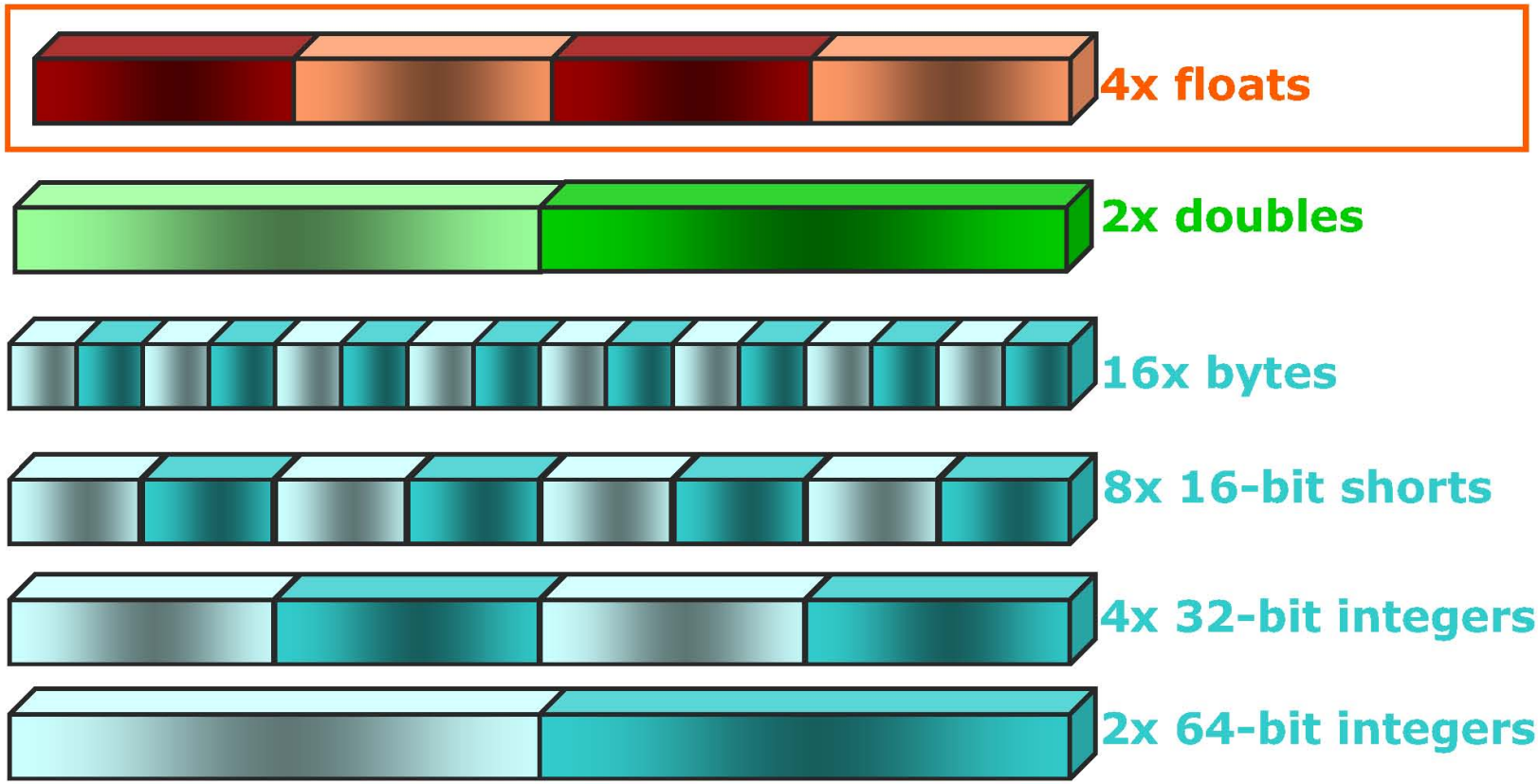
```
kernel void Fct(float a<>, float b<>, out float c<>) {
   c = a + b;
 }
int main(int argc, char** argv) {
   int i, j;
   float a<10, 10>, b<10, 10>, c<10, 10>;
   float input_a[10][10],input_b[10][10], input_c[10][10];
  for(i=0; i<10; i++) {
     for(j=0; j<10; j++) {
      input_a[i][j] = (float) i;
      input_b[i][j] = (float) j;
    }
  }
 streamRead(a, input_a);
 streamRead(b, input_b);
 Fct(a, b, c);
 streamWrite(c, input_c);
 ...
}
```

Brook+ example



SSE Data types

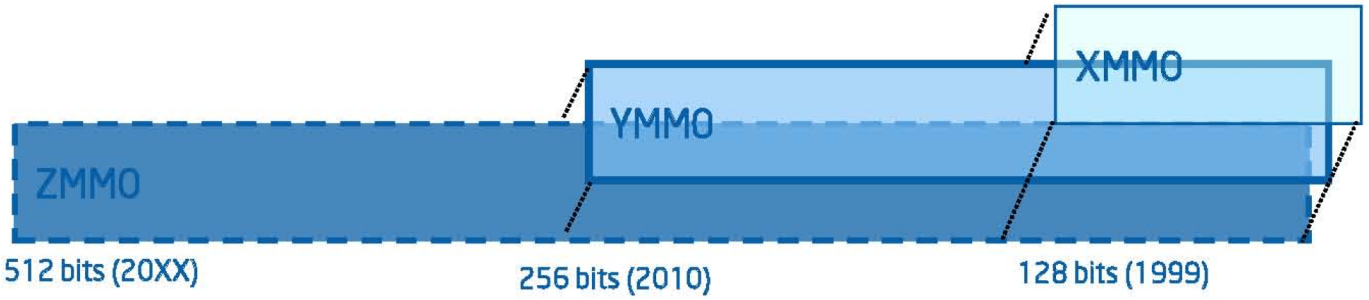
128 bit word (XMM)

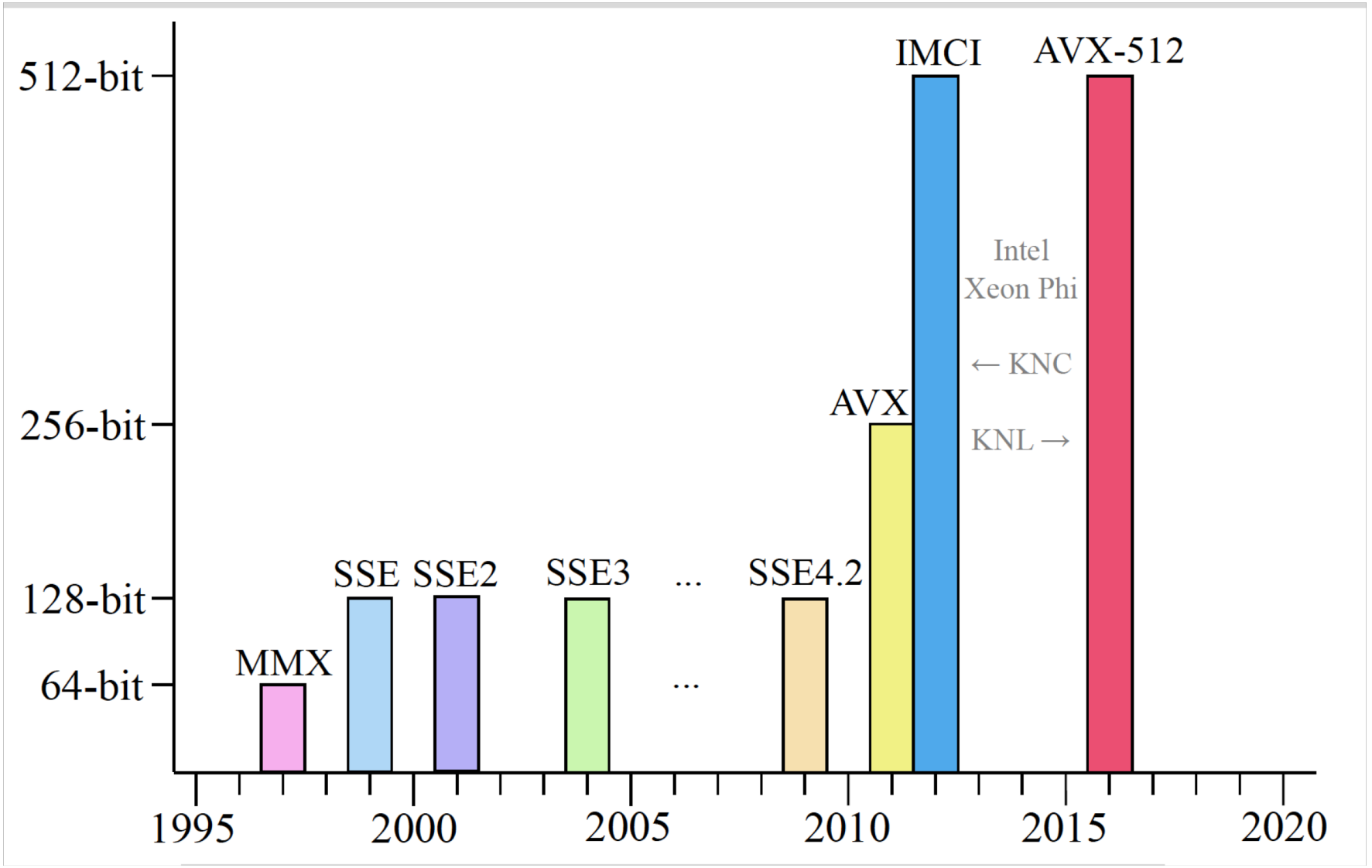


Sandy Bridge (2010): Intel® AVX

A 256-bit vector extension to SSE

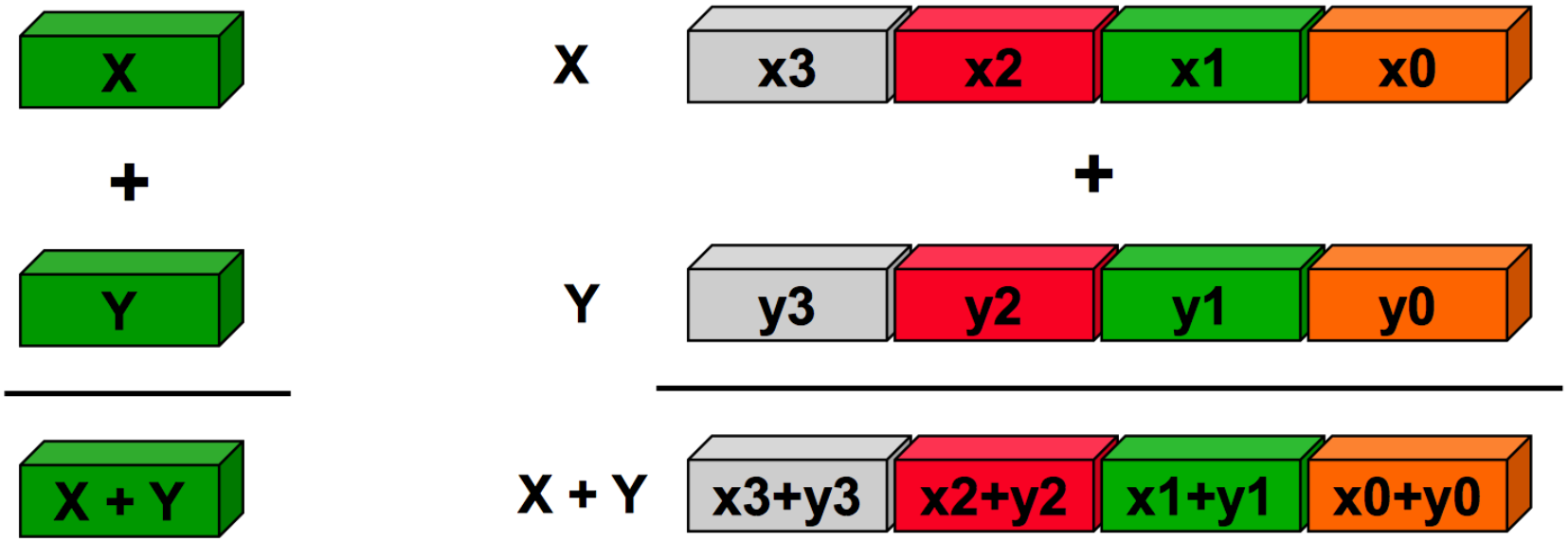
- Intel® AVX extends all 16 XMM registers to 256bits
- Intel® AVX works on either
  - The whole 256-bits
  - The lower 128-bits(like existing SSE instructions)
    - A drop-in replacement for all existing scalar/128-bit SSE instructions
- The new state extends/overlays SSE
- The lower part (bits 0-127) of the YMM registers is mapped onto XMM registers




512-bit
256-bit
128-bit
64-bit
MMX
SSE
SSE2
SSE3
...
...
SSE4.2
AVX
IMCI
AVX-512
Intel
Xeon Phi
← KNC
KNL →
1995
2000
2005
2010
2015
2020

Single Instruction Multiple Data

- Scalar processing
  - traditional mode
  - one operation produces one result
- SIMD processing (Intel)
  - with SSE / SSE2
  - one operation produces multiple results



Slide Source: Alex Klimovitski & Dean Macri, Intel Corporation

Single Instruction Multiple Data

- SLP (Superword Level Parallelism)
  - Direct mapping to underling SIMD machine instruction
  - Usually implemented using array/vector notation
- Loop Vectorization
  - Transform a loop into N streams (N=SIMD-width)
  - Compiler assisted or implemented in a "vector-library"
- Loop vectorization is more efficient than SLP
  - Transform your problem in a long loop over simple quantities

“Vector Extension”

- SIMD vector can be found implemented as compiler’s extension or libraries
  - https://gcc.gnu.org/onlinedocs/gcc/Vector-Extensions.html
  - http://clang.llvm.org/docs/LanguageExtensions.html#vectors-and-extended-vectors
  - http://www.cilkplus.org/tutorial-array-notation
  - http://code.compeng.uni-frankfurt.de/projects/vc
- Here we will experiment with “gcc vectors”

Gcc Vector extension

```
typedef T __attribute__( ( vector_size( N*sizeof(T) ) ) ) VecNT;

typedef float __attribute__( ( vector_size( 16 ) ) ) Vec4F;
Vec4F a{0,1f,-2f,3f}, b{-1f,-2f,3f,0}, c{0,2.f,4.f,5.f}, zero{0};

c += 3.14f*b*a;
auto z = (a>0) ? a : -a;
auto m = (a>b) ? a : b;
auto t = a/b; t = (x>pi/8.f) ? (t-1.0f)/(t+1.0f) : t;
```

Vector of integers: 0 for false, -1 for true

always computed

- scalar code: if(x>pi/8.f) t= (t-1.0f)/(t+1.0f) ;

“Auto” vectorization

- The process that transform scalar code in vector code
- As a compiler pass
  - Issues: detect and manage data dependencies
  - Hints from user as macro
- OpenMP4
  - New: implementations still experimental
  - icc: “fully supported?”
  - gcc: syntax and code generation ok, vectorization relies on the corresponding compiler pass
- OpenCL:
  - Uses compiler backend

Loop Vectorization

More at http://gcc.gnu.org/projects/tree-ssa/vectorization.html

- original serial loop:

```
for(i=0; i<N; ++i){
   a[i] = a[i] + b[i];
}
```

vectorization

- loop in vector notation:

```
for (i=0; i<N/4; ; i+=4){
   V4& va = *((V4*)a[i]);
    va  +=   *((V4 const *)b[i]);
} vectorized loop (4 times less iterations)
```

- loop in vector notation:

```
for (i=0; i<(N-N%4); i+=4){
   V4& va = *((V4*)a[i]);
    va  +=   *((V4 const *)b[i]);
}    vectorized loop

for ( ; i < N; i++) {
  a[i] = a[i] + b[i];
}       epilog loop
```

- Loop based vectorization
- No dependences between iterations

Loop Dependences

```
for (i=0; i<N; ++i){
      A[i+1] = B[i] + X
      D[i] = A[i] + Y
}
```

```
for (i=0; i<N; ++i)
      A[i+1] = B[i] + X

for (i=0; i<N; ++i)
      D[i] = A[i] + Y
```

```
for (i=0; i<N; ++i){
      B[i] = A[i] + Y
      A[i+1] = B[i] + X
}
```

```
for (i=0; i<N; ++i){
      B[i] = A[i] + Y
      A[i+1] = B[i] + X
}
```

```
for (i=0; i<N; ++i)
      for (j=0; j<N; ++j)
          A[i+1][j] =  A[i][j] + X
```

Subtle issues:
A may partially overlap
  with B
  with X
  with N
The compiler will generate runtime checks and alternative sequential code.
To avoid this overhead use local variable, "restrict" keyword or #pragma GCC ivdep

```
void ignore_vec_dep (int *a, int k, int c, int m)
{
#pragma GCC ivdep
    for (int i = 0; i < m; ++i)
      a[i] = a[i + k] * c;
}
```

Reduction

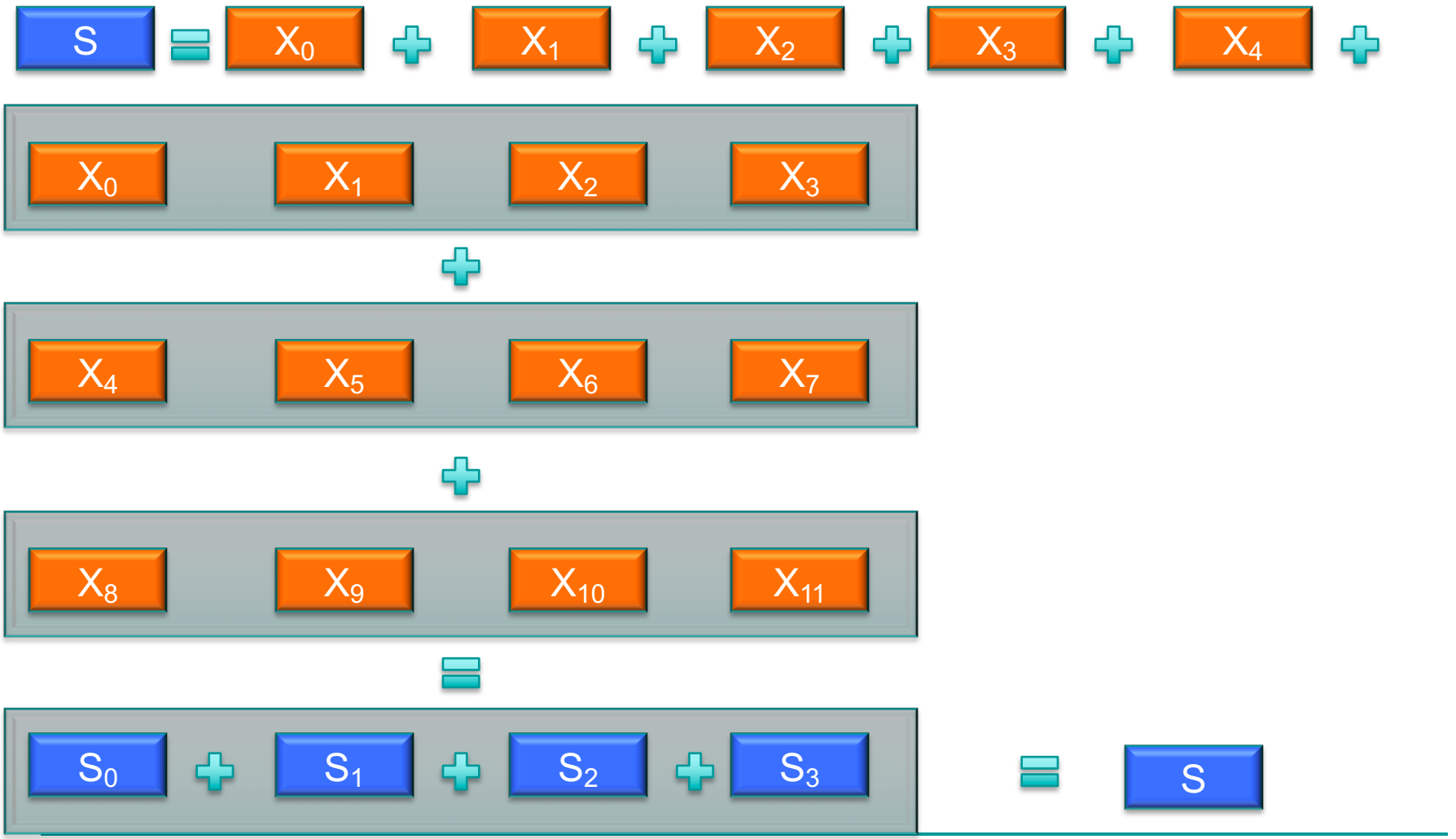
```
float innerProduct() {
   float s=0;
   for (int i=0; i!=N; i++)
      s+= a[i]*b[i];
   return s;
}
```

```
// pseudo code
float innerProduct() {
   V4 s ={0};
   for (int i=0; i<N/4; ++i)
     s += *((V4 const *)a[i]) *  *((V4 const *)b[i]);

   // horizontal sum;
   float sum=s[0];
   for (int j=1;j!=4;++j)sum+=s[j];
   return sum;
}
```

Requires *relaxed* float-math rules
(-Ofast)

Reduction



Real code http://goo.gl/3ku9EJ

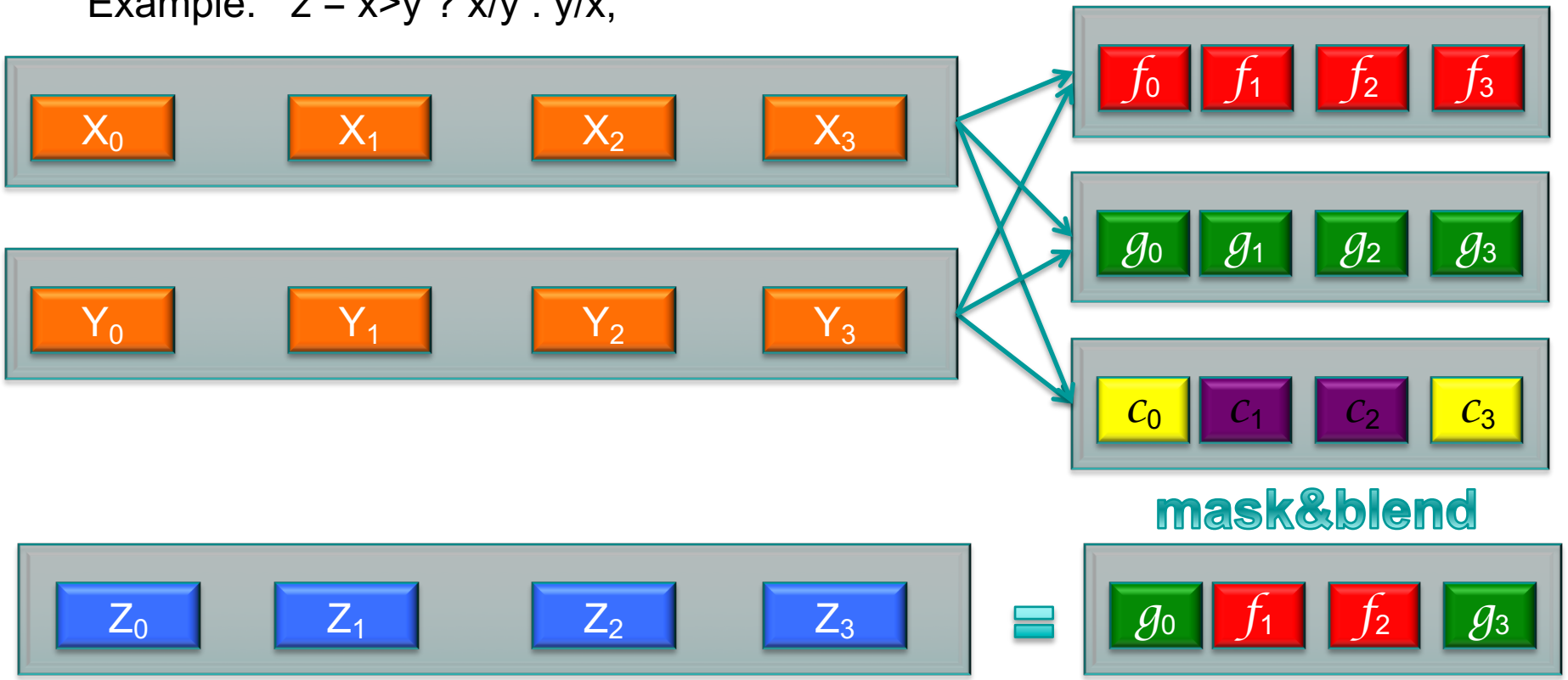
```
float a[1024],b[1024]; int N=1024;
float innerProduct() {
   float s=0;
   for (int i=0; i!=N; i++)
      s+= a[i]*b[i];
   return s;
}
```

```
.L3:
        movss   a(%rax), %xmm1
        addq    $4, %rax
        mulss   b-4(%rax), %xmm1
        addss   %xmm1, %xmm0
        cmpq    %rdx, %rax
        jne     .L3
```

```
.L4:
        movaps  b(%rsi), %xmm1
        addl    $1, %edi
        addq    $16, %rsi
        mulps   a-16(%rsi), %xmm1
        addps   %xmm1, %xmm0
        cmpl    %edi, %edx
        ja      .L4
        haddps  %xmm0, %xmm0
        haddps  %xmm0, %xmm0
        cmpl    %ecx, %eax
        je      .L15
```

Conditional Code

Example: z = x>y ? x/y : y/x;



Conditional code : https://godbolt.org/g/shCUuE

```
double x[1024],y[1024] ,z[1024]; int N=1024;
void foo() {
   for (int i=0; i!=N; i++) {
      if (x[i]>y[i]) z[i]=x[i]/y[i];
      else z[i]=y[i]/x[i];
  } // exercise: write it with only one division
}
```

loop in vector notation:

```
for (i=0; i<N/4; ++i){
 V4 vx = &((V4 const *)x[i]);
 V4 vy = &((V4 const *)y[i]);
 V4 & vz = *((V4 *)z[i]);
  I4 t = vx > vy;
 // compute both branches
  auto a  = vx / vy;  auto b = vy / vx;
 // mask and "blend"
  vz = t ? a : b;
}
```

```
foo():
        xorl    %eax, %eax
.L2:
        movapd  x(%rax), %xmm2
        addq    $16, %rax
        movapd  y-16(%rax),
%xmm0
        movapd  %xmm2, %xmm3
        divpd   %xmm0, %xmm3
        movapd  %xmm0, %xmm1
        cmpltpd %xmm2, %xmm0
        divpd   %xmm2, %xmm1
        blendvpd %xmm0, %xmm3,
%xmm1
        movaps  %xmm1, z-
16(%rax)
        cmpq    $8192, %rax
        jne     .L2
        ret
```

The compiler is able to make the transformation of a condition in *"compute, mask and blend"* if code is not too complex

Vectorization of "math function"

- Currently linux libm does not support vectorization
- Exploit compiler + vendor libraries
  - Requires licensed libs by intel and/or amd
  - No change in user code: just recompile
    - -mveclibabi=svml –L/…/lib/intel64 -lsvml -lirc
    - -mveclibabi=acml –L/…/lib/amd64 -lacml –lamdlibm
- Exploit auto-vectorization
  - Modified cephes library (or other open source)
    - Requires header-file + different function names
  - Look into vdt/ (https://svnweb.cern.ch/trac/vdt)
    - Project for a student: port vdt to gcc simd-vectors
  - For your exercise use SimpleSinCos.h
    - simpleSin(x), simpleCos(x), simpleSinCos(x,s,c)

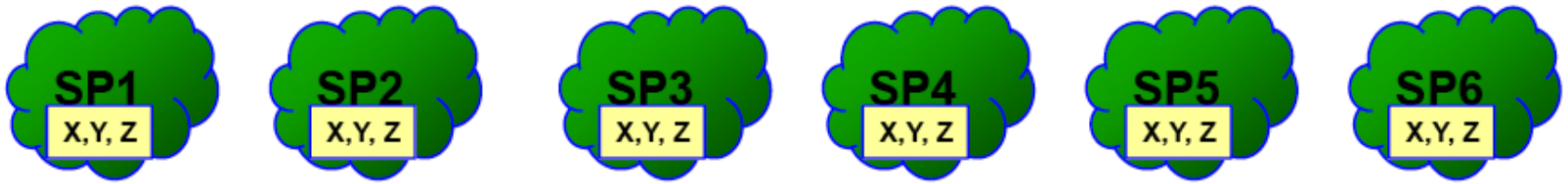
https://github.com/CppCon/CppCon2014/tree/master/Presentations/Data-Oriented%20Design%20and%20C%2B%2B

http://aras-p.info/texts/files/2018Academy%20-%20ECS-DoD.pdf

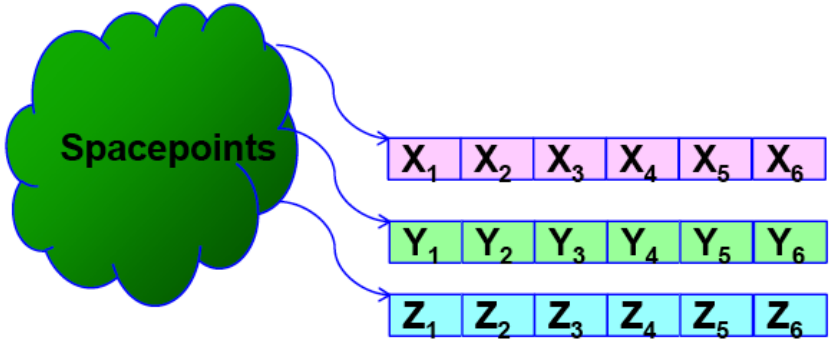
DATA ORGANIZATION

Data Organization: AoS vs SoA

- Traditional Object organization is an Array of Structures
  - Abstraction often used to hide implementation details at object level



- Difficult to fit stream computing
- Better to use a Structure of Arrays
  - (column-wise storage)
- OO can wrap SoA as the AoS
  - Move abstraction higher
  - Expose data layout to the compiler



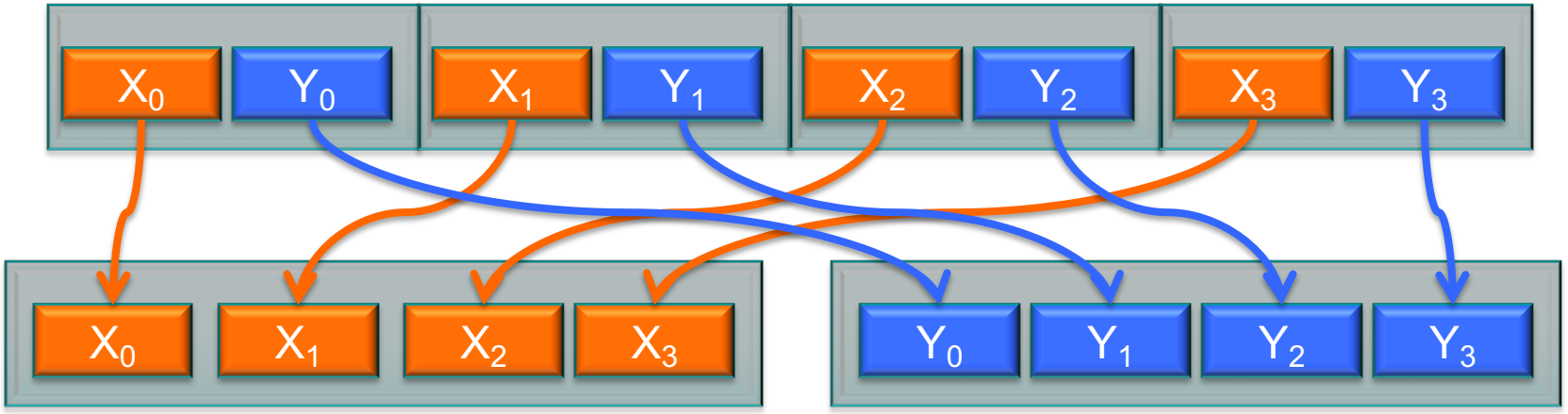
- Explicit copy in many cases more efficient
  - (notebooks vs whiteboard)

AoS vs SoA

```
struct Point {
  float x,y,z;
};
struct Points {
  std::vector<Point> p;
};
```

```
struct Points {
  std::vector<float> x,y,z;
};
```

The choice of AoS vs SoA depends on the access patterns in the application
Operations on AoS can be vectorized at the cost of *shuffles* or *permutations*
For large structures this becomes not profitable pretty fast.
In general SoA shall be preferred to fully exploit vectorization

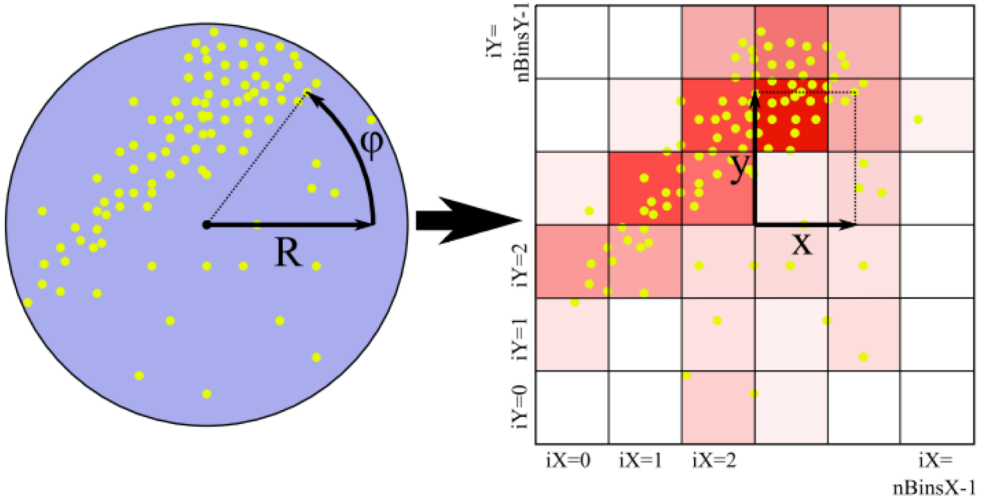


Don't stop the stream!

- Vector code is effective as long as
  - We do not go back to memory
    - Operate on local registries as long as possible
  - We maximize the number of useful operations per cycle
    - Conditional code is a killer!
    - Better to compute all branches and then blend
- Algorithms optimized for sequential code are not necessarily still the fastest in vector
  - Often slower (older…) algorithms perform better

Excercise

https://infn-esc.github.io/esc16/vectorization/binning.html



Take points in polar coordinates
Fill a two dimensional cartesian Histogram

```
struct Point { float phi,r; };
struct Points {
   std::array<Point,N> p;
 };
Points points;
constexpr int NBin = 100;
struct Hist {
 int bin[NBin+1][NBin+1] = {0};
};
float binWidth = 2./NBin;
Hist h;
```

```
For(auto const & p : points.p) {
  auto x = p.r*std::cos(p.phi);
  auto y = p.r*std::sin(p.phi);
  int xbin = (x+1.f)/binWidth;
  int ybin = (y+1.f)/binWidth;
  assert(xbin>=0 && ybin>=0);
  assert(xbin<101 && ybin<101);
  ++h.bin[xbin][ybin];
 }
```

Exercise 1

- Open SimpleVectorization.cc
  http://goo.gl/SAiici
- Compile it with 03, Ofast, more fancy options
  - Analyze the compiler report
    - Correlate with code and generated instruction
    - Is vectorizing everything?
    - (if too complex, comment-out all but one function)
    - Add ” -fopt-info-vec”
    - Try “-fopt-info-vec-missed -fno-tree-slp-vectorize”

objdump -S -r -C --no-show-raw-insn –w xyz.o | less

build SimpleVectorization_vect.s;

cat SimpleVectorization_vect.s| less

Exercise 2

https://infn-esc.github.io/esc18/vectorization/pi.html

- Open pi.cpp http://goo.gl/zI3WqS
  - Compile it with -02, -Ofast, more fancy options
  - Change double in float
  - Try to vectorize using native vectors…

Pi Program: Vectorization with intriniscs (SSE)

See https://software.intel.com/sites/landingpage/IntrinsicsGuide/

```
 float pi_sse(int  num_steps)
{  float scalar_one =1.0, scalar_zero = 0.0,  ival, scalar_four =4.0, step, pi, vsum[4];
   step = 1.0/(float) num_steps;

   __m128 ramp   = _mm_setr_ps(0.5, 1.5, 2.5, 3.5);
   __m128 one    = _mm_load1_ps(&scalar_one);
   __m128 four   = _mm_load1_ps(&scalar_four);
   __m128 vstep  = _mm_load1_ps(&step);
   __m128 sum    = _mm_load1_ps(&scalar_zero);
   __m128 xvec;   __m128 denom;  __m128 eye;

  for (int i=0;i< num_steps; i=i+4){          // unroll loop 4 times
     ival       = (float)i;                   // and assume num_steps%4 = 0
     eye        = _mm_load1_ps(&ival);
     xvec       = _mm_mul_ps(_mm_add_ps(eye,ramp),vstep);
     denom  = _mm_add_ps(_mm_mul_ps(xvec,xvec),one);
     sum      = _mm_add_ps(_mm_div_ps(four,denom),sum);
   }
   _mm_store_ps(&vsum[0],sum);
   pi = step * (vsum[0]+vsum[1]+vsum[2]+vsum[3]);
  return pi;
}   // credit T.M.
```