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High-performance Scientific Computing in C++

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Introduction

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- Specify actions to be executed by the machine

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C++ is a language for developing and using elegant and efficient abstractions

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- Leave no room for a lower level language
- What you don't use, you don't pay for

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C++ in scientific computing

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  - Hardware aware translation of ideas into code
  - Profiling and tuning

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Know your hardware

Warm up!

Get your session ready!

- We will use the following shorthands:

```
G = g++ -O3 -pedantic -Wall \
      -std=c++14
A = clang++ -O3 -pedantic -Wall \
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```

- Go to `examples` and open `warmup.cc`
- Compile using our short cut : `G warmup.cc`.

```
int main()
{
  auto  high = 100'000'000.0f;
  auto low = 99'999'990.0f;
  do {
    std::cout << high << "\n";
    high -= 1;
  } while (high > low);
}
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- Ready ?

Floating point numbers

Area of a triangle of sides a, b and c...

- Heron's formula (Metrica, Heron of Alexandria, ≈ 60 CE)

$$
\begin{aligned}
s &= \frac{a+b+c}{2} \\
\Delta &= \sqrt{s \times (s-a) \times (s-b) \times (s-c)}
\end{aligned}
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- Kahan's formula (Miscalculating Area and Angles of a Needle-like Triangle, W. Kahan, 2000 CE, http://http.cs.berkeley.edu/~wkahan/Triangle.pdf)

$$\begin{aligned} a \geq b &\geq c \\ \Delta &= \frac{1}{4}\sqrt{(a+(b+c)) \times (c-(a-b)) \times (c+(a-b)) \times (a+(b-c))} \end{aligned}$$

Floating point numbers

```
const auto a = 5.0f;
const auto b = 4.0f;
const auto c = 3.0f;
std::cout << "Heron's formula = "
      << area_heron(a,b,c) << "\n";
std::cout << "Kahan's formula = "
      << area_kahan(a,b,c) << "\n";
```

```
Heron's formula = 6
Kahan's formula = 6
```

- Mathematically, both calculate the same thing

Example 1:

`examples/area.cc` contains an implementation of both these formulae. Change the sides of the triangles a few times. Try the values in the commented out lines.

See also: CppCon 2015: John Farrier "Demystifying Floating Point"

Floating point numbers

```
const auto a = 100'000.000'00f;
const auto b =  99'999.999'79f;
const auto c =       0.000'29f;
std::cout << "Heron's formula = "
      << area_heron(a,b,c) << "\n";
std::cout << "Kahan's formula = "
      << area_kahan(a,b,c) << "\n";
```

```
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- If the triangle becomes very long and thin though, weird things happen

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- If the triangle becomes very long and thin though, weird things happen
- Correct answer is 10.

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Representation of floating point numbers

$$-1^{s} \times 1.mantissa \times 2^{exponent}$$

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- For a fixed exponent, there are 2^{23} different floating point numbers. $\implies$ There are as many **`float`**s between 2^{-11} and 2^{-10} as there are between 1024 and 2048
- By contrast, integral types have a uniform density throughout their range

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- To maintain our sanity, we will write it as
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- Mental exercise: we have two decimal numbers in scientific notation 9.78×10^2, and 1.0×10^{-1}. How will you add them ?
- You shift the decimal point in one of them until the exponents are the same, and then add the mantissas: $9.78 \times 10^2 + 0.001 \times 10^2$. Digits in the smaller number are pushed to the right

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- What is 2.0 ? $[0][(2^1)][00000000000000000000000]$. What if you add these two ? What information about the smaller number can we retain ?

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- This quantity depends on the floating point type. In C++, you can retrieve it `std::numeric_limits<T>::epsilon()`
- Two quantities with exponent 0 can not be distinguished in this representation, if they differ by less than `epsilon`
- In an expression like `(big+small)-big`, if `big` and `small` differ by more than 23 in exponent, all information about `small` is lost, and we get a 0. $2^{23} = 8388608$.

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- Not enough bits to represent such small quantities.
- All exponent bits being 1 indicate some special “numbers”:
  - $\pm\infty$: all mantissa bits 0.
  - NaN : at least one mantissa bit non-zero.

Example 2:

In `examples/floating_fun.cc`, there is a small program "simulating" a calculation involving some large quantities adding up to 0. Eight numbers are stored in an array of floats, and their sum evaluated and printed. The calculation is repeated by permuting the indexes of the array, so that the nubmers are added in all possible orders. Observe the output!

Exercise 1: std::numeric_limits

What is epsilon for **`float`** and **`double`** on your computer ? Find out by writing a small C++ program and printing out the values from `std::numeric_limits`. Look up the documentation of `numeric_limits`. What other information can you get about numeric types from that header ?

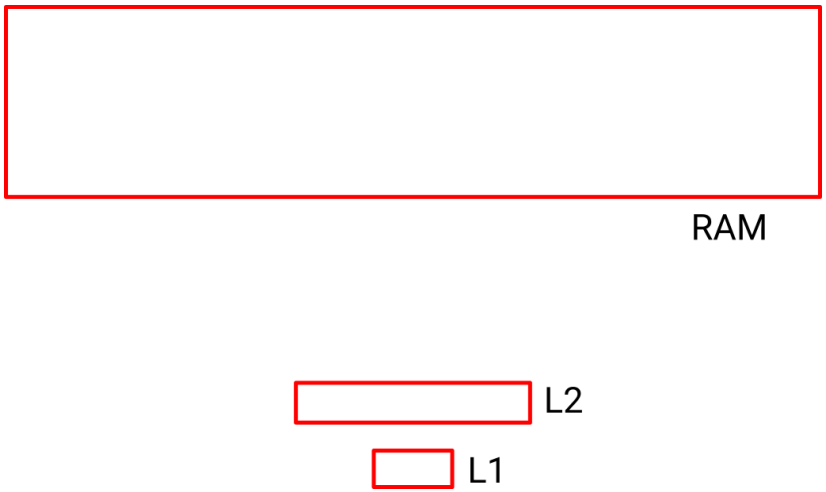
Float: $[1-\text{bit}][8-\text{bits}][23-\text{bits}]$

Maximum	3.40282e+38
Minimum	1.17549e-38
Lowest	-3.40282e+38
Epsilon	1.19209e-07
Rounding error	0.5

Double: $[1-\text{bit}][11-\text{bits}][52-\text{bits}]$

Maximum	1.79769e+308
Minimum	2.22507e-308
Lowest	-1.79769e+308
Epsilon	2.22045e-16
Rounding error	0.5

Memory



- Cost of fetching one integer from the main memory can be a hundred times larger than getting it from the L1 cache
- Fun fact: in 1 clock cycle of the CPU on my laptop, a photon travels about 10 cm!

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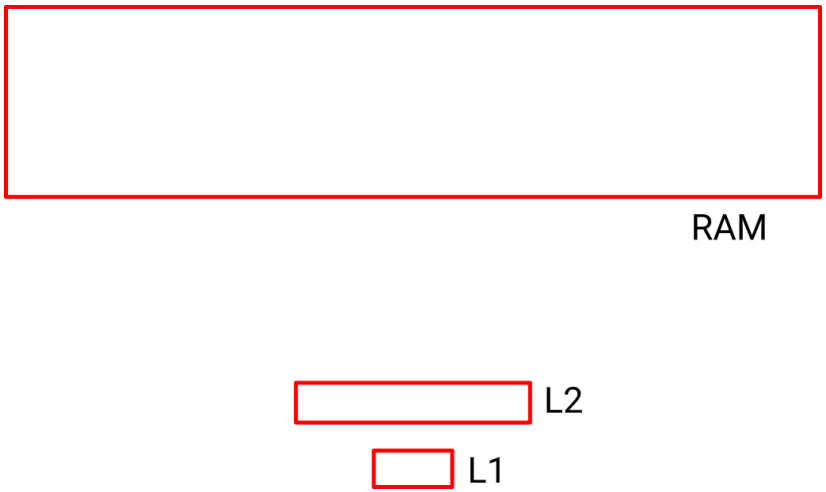

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- Memory is fetched in “cache lines”
- Successive operations on contiguous memory locations do not incur the full cost of main memory access

Memory

```
std::vector<int> A(N*N, 0.0);
for (size_t i=0; i<N; ++i) {
    for (size_t j=0; j<N; ++j) {
        A[i*N+j] += j+i;
    }
}
```

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```
for (size_t i=0; i<N*N; ++i) {
    A[pos[i]] += i;
}
```

- Q: Which way of accessing the "matrix" is faster, and by how much ?

See also: CppCon 2016: Timur Doumler "Want fast C++? Know your hardware!"

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- Q: Which way of accessing the "matrix" is faster, and by how much ?
- A: For N=10000, my laptop takes about 0.046 seconds for the row major pattern (top), and about 1.14 seconds for the column major pattern (middle), and 1.9 seconds for random pattern (bottom)

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Memory

```
constexpr size_t size = 2 << 26;
std::vector< long > A(size, 0);
for (size_t step = 1; step <= 2048; step *= 2) {
  for (size_t i = 0; i < size; i += step) A[i]++;
}
```

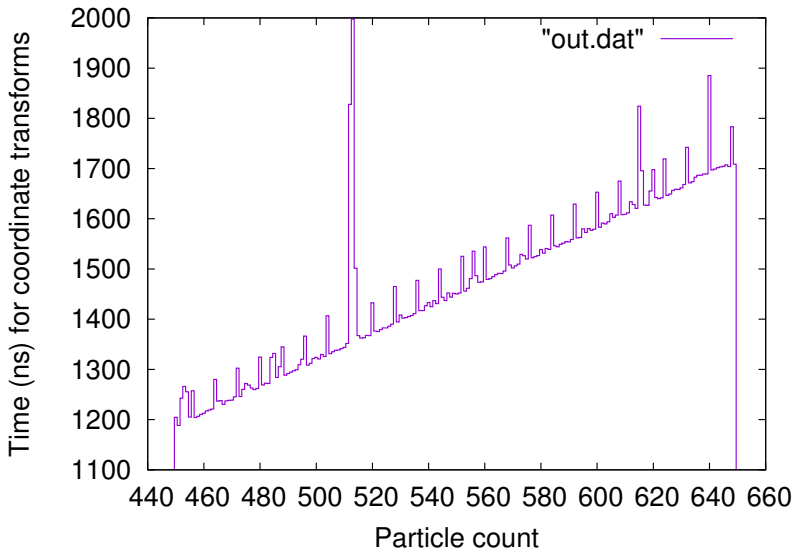
Step	Time
1	0.128
2	0.121
4	0.120
8	0.121
16	0.112
32	0.075
64	0.029
128	0.015
256	0.008
512	0.004
1024	0.003
2048	0.001

- For small step sizes, increasing the number of writes to the array does not change the total time.
- Multiple accesses inside a cache line has minimal extra cost.

4K aliasing

```
// Layout :
// x0, x1, x2 ... xn-1, y0, y1 ... yn-1,
// z0, z1 ... zn-1, wx0, wx1 ... wxn-1,
// wy0, wy1 ... wyn-1, wz0 ... wzn-1

for (size_t i=0;i<npart;++i) {
  world_x(i,R(0,0)*x(i)+R(0,1)*y(i)
           +R(0,2)*z(i));
  world_y(i,R(1,0)*x(i)+R(1,1)*y(i)
           +R(1,2)*z(i));
  world_z(i,R(2,0)*x(i)+R(2,1)*y(i)
           +R(2,2)*z(i));
}
```



- Innocent looking code can sometimes produce weird changes in performance based on array sizes
- The spike in required time here comes for a particle count of about 512, when the different components of the data for one particle are separated by exactly 4kB.

Example 3: examples/memory_effects

In the folder `examples/memory_effects` you will find a few small programs illustrating the cache effects discussed so far:

- `traverse0.cc` can be used to compare contiguous and non-contiguous access of a large array
- `every_nth.cc` compares times for accessing every n'th element, and highlights the cache line
- `traverse1.cc` compares contiguous and non-contiguous access for different array sizes
- `war.cc` illustrates unexpected cache misses in regularly arranged data

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- Organise code to maximise the use of any cache line that has been fetched:
  - Collate processing of nearby memory locations
  - Organise data structures so that things processed together are also stored near each other
- Keep variables as local as possible

Functions

```
return_type function_name(parameters)
{
  // function body
}
double sin(double x)
{
  // Somehow calculate sin of x
  return answer;
}
int main()
{
  constexpr double pi=3.141592653589793;
  for (int i=0;i<100;++i) {
    std::cout << i*pi/100
       << sin(i*pi/100) <<"\n";
  }
  std::cout << sin("pi") <<"\n"; //Error!
}
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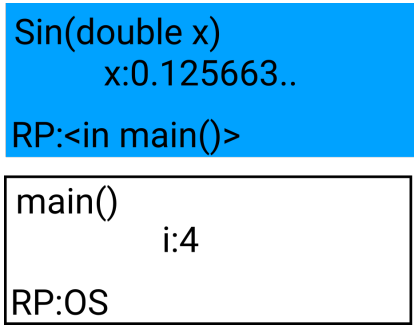
- A function must be called with values called "arguments".
- The type of the arguments must match or be implicitly convertible to the corresponding type in the function parameter list

Functions at run time

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```

- When a function is called, it is given a "workbook" in memory called a stack frame
- Arguments are copied to registers or the stack as well as a return address
- (Non-static) local variables are allocated in the stack
- When the function concludes, execution continues at the return address, and the stack frame is destroyed

Recursion

- SP=<in someother()> RP=<...>

```
1  unsigned int factorial(unsigned int n)
2  {
3    int u=n; // u: Unnecessary
4    if (n>1) return n*factorial(n-1);
5    else return 1;
6  }
7  int someother()
8  {
9    factorial(4);
10 }
```

- Stack frame is bound to an individual call, not to the function body
- Each level of "recursion" has its own stack frame

Recursion

- SP=<in factorial()> n=4 u=4 RP=<9>
- SP=<in someother()> RP=<...>

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9    factorial(4);
10 }
```

- Stack frame is bound to an individual call, not to the function body
- Each level of "recursion" has its own stack frame
- Function parameters are copied to the stack frame

Recursion

- SP=<in factorial()> n=3 u=3 RP=<4>
- SP=<in factorial()> n=4 u=4 RP=<9>
- SP=<in someother()> RP=<...>

```
1  unsigned int factorial(unsigned int n)
2  {
3    int u=n; // u: Unnecessary
4    if (n>1) return n*factorial(n-1);
5    else return 1;
6  }
7  int someother()
8  {
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10 }
```

- Stack frame is bound to an individual call, not to the function body
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- Local variables at different levels of recursion live in their own stack frames, and do not interfere

Recursion

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- SP=<in factorial()> n=3 u=3 RP=<4>
- SP=<in factorial()> n=4 u=4 RP=<9>
- SP=<in someother()> RP=<...>

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2  {
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Recursion

- SP=<in factorial()> n=1 u=1 RP=<4>
- SP=<in factorial()> n=2 u=2 RP=<4>
- SP=<in factorial()> n=3 u=3 RP=<4>
- SP=<in factorial()> n=4 u=4 RP=<9>
- SP=<in someother()> RP=<...>

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Recursion

- SP=<in factorial()> n=4 u=4 RP=<9>
- SP=<in someother()> RP=<...>

```
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- Each level of "recursion" has its own stack frame
- Function parameters are copied to the stack frame
- Local variables at different levels of recursion live in their own stack frames, and do not interfere

Functions: under the microscope!

```
double f(const double x, const double y)
{
    return x+y*y;
}
```

```
# G="g++ -std=c++14 -march=Native -O3"
G -c -g f.cc
objdump -d -M intel -S f.o
```

```
0000000000000000 <_Z1fdd>:
  vmulsd xmm1,xmm1,xmm1
  vaddsd xmm0,xmm1,xmm0
  ret
```

- Function parameters are passed in registers or copied to the stack

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- Function parameters are passed in registers or copied to the stack
- On X86_64 under Linux,
  - XMM0..XMM7 are used for floating point arguments

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double f(const double x, const double y)
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```

```
0000000000000000 <_Z1fdd>:
  vmulsd xmm1,xmm1,xmm1
  vaddsd xmm0,xmm1,xmm0
  ret
```

- Function parameters are passed in registers or copied to the stack
- On X86_64 under Linux,
  - XMM0..XMM7 are used for floating point arguments
  - 6 integer or pointer arguments are passed in registers RDI, RSI, RDX, RCX, R8 and R9

Functions: under the microscope!

```
class D {
  int nm;
  double d;
public:
  inline void val(double x) { d=x; }
  inline double val() const { return d; }
  inline auto name() const { return nm; }
  double operator+(double x1) const;
};
```

```
double D::operator+(double x) const
{
    return d+x*x;
}
```

```
0000000000000000 <_ZNK1DplEd>:
  vmulsd xmm0,xmm0,xmm0
  vaddsd xmm0,xmm0,QWORD PTR [rdi+0x8]
  ret
```

- Object of different classes are passed as pointers (references are hidden pointers)
- Any additional arguments are passed on the stack
- Function body is executed
- Return value is written
- Execution continues at the previously stored return address

Stack

```
class V3 {
  double x,y,z;
  V3 cross(const V3 &);
  double dot(const V3 &);
};
double prob(int i, const V3 & x,
            const V3 & y)
{
  int j=i%233;
  V3 tmp{x};
  for (;j<i;++j) {
    tmp=tmp.cross(y);
  }
  return tmp.dot(x);
}
```

- Heavily reused memory locations

Stack

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class V3 {
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```

- Heavily reused memory locations
- Likely cached, therefore, fast

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  for (;j<i;++j) {
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  return tmp.dot(x);
}
```

- Heavily reused memory locations
- Likely cached, therefore, fast
- All local variables of any type

Global storage

```
double prob(int i)
{
  static int c{0};
  ++c;
  if (c%1000==0) {
    std::cout<<"Call count reached "
      << c << "\n";
  }
  static const double L[]={3.14,2.71};
  return L[i%2];
}
```

- Variables outside any function

Global storage

```
double prob(int i)
{
  static int c{0};
  ++c;
  if (c%1000==0) {
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- Variables outside any function
- Variables marked with the **`static`** keyword in functions

Global storage

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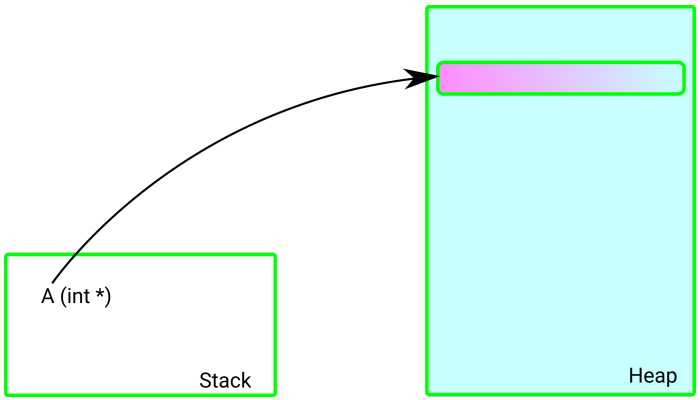
  }
  static const double L[]={3.14,2.71};
  return L[i%2];
}
```

- Variables outside any function
- Variables marked with the **`static`** keyword in functions
- Floating point constants, array initializer lists, jump tables, virtual function tables

Heap

```
void f()
{
  int *A=new int[1000000];
  // calculations with A
  delete [] A;
}
```



- Explicitly/implicitly managed memory through **`new`**, **`delete`**, `malloc` or `free`

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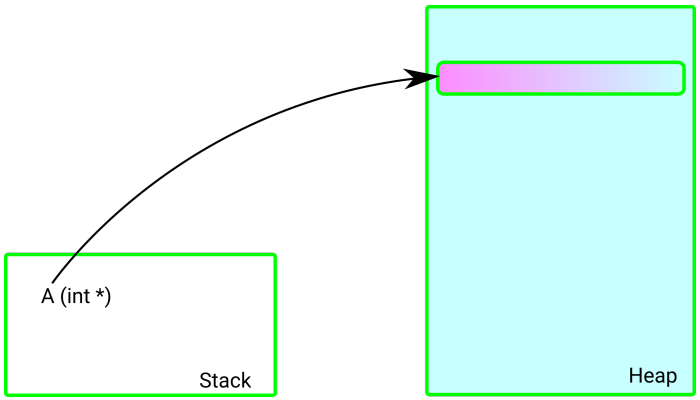

- Explicitly/implicitly managed memory through **`new`**, **`delete`**, `malloc` or `free`
- Can store very large objects which don't fit in the stack

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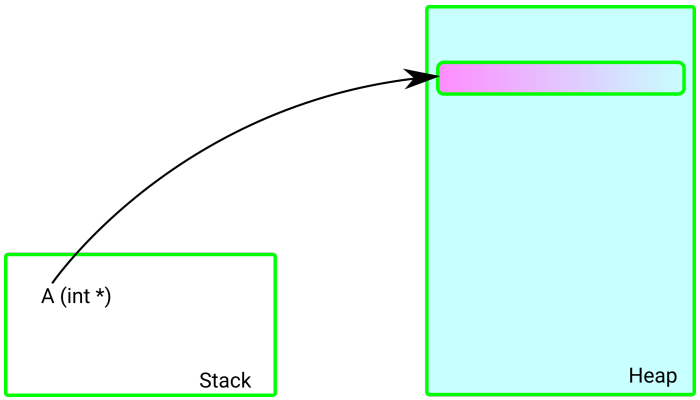

- Explicitly/implicitly managed memory through **`new`**, **`delete`**, `malloc` or `free`
- Can store very large objects which don't fit in the stack
- Arrays whose size is not known at compile time. C99 style variable length arrays are not standard C++.

Heap

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void f()
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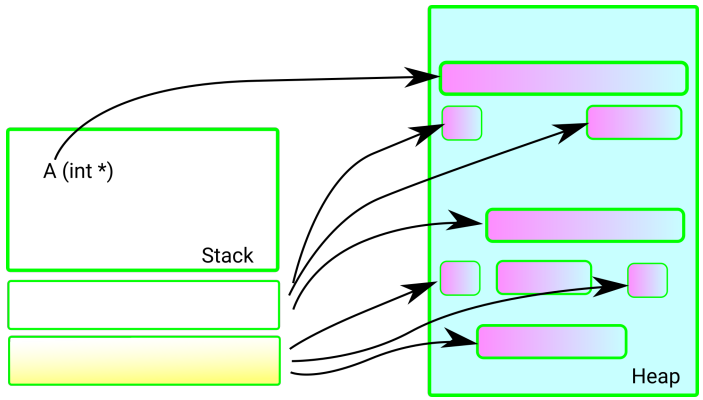
```



- Tends to get fragmented

Heap

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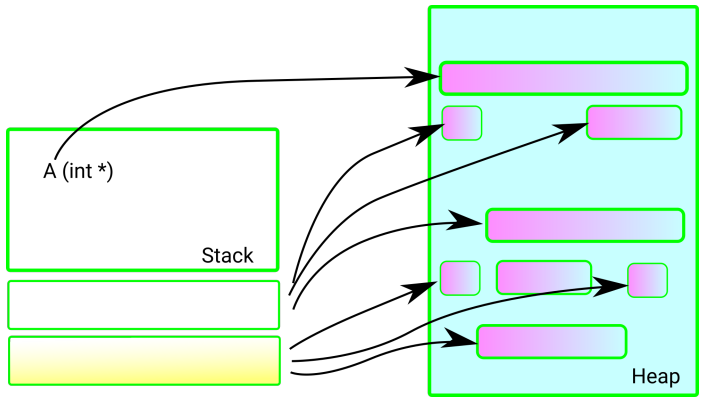

- Tends to get fragmented
- Must find a suitably sized unused block

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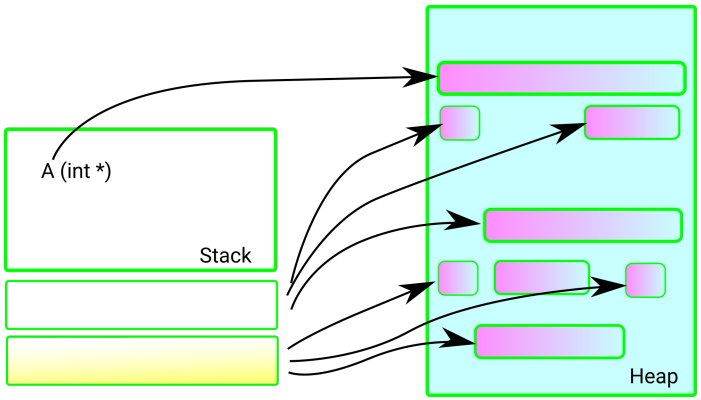

- Tends to get fragmented
- Must find a suitably sized unused block
- Must keep track of what is and isn't in use

Heap

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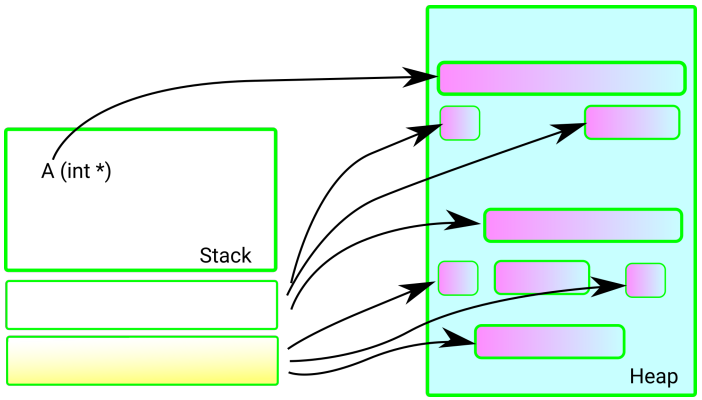

- Tends to get fragmented
- Must find a suitably sized unused block
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- Must remember to free memory before accessing pointers go out of scope

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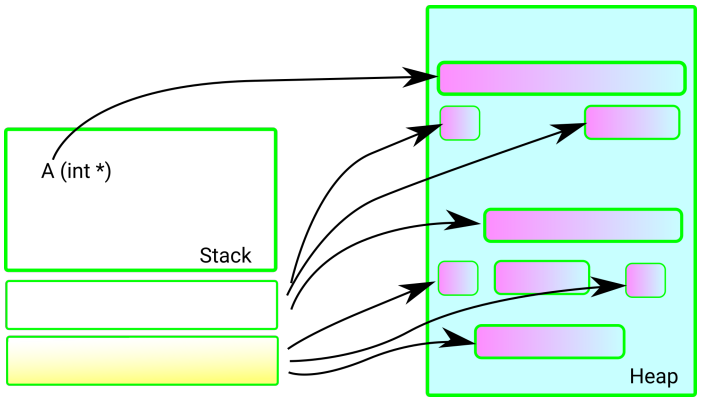

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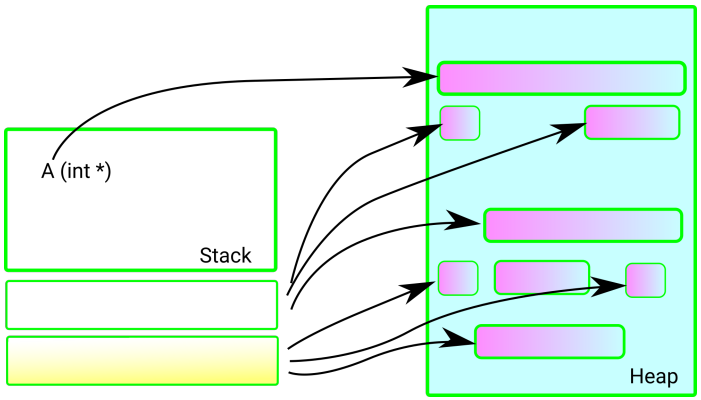


- Tends to get fragmented
- Must find a suitably sized unused block
- Must keep track of what is and isn't in use
- Must remember to free memory before accessing pointers go out of scope
- Objects stored one after the other may end up in very different locations
- Slower than stack storage

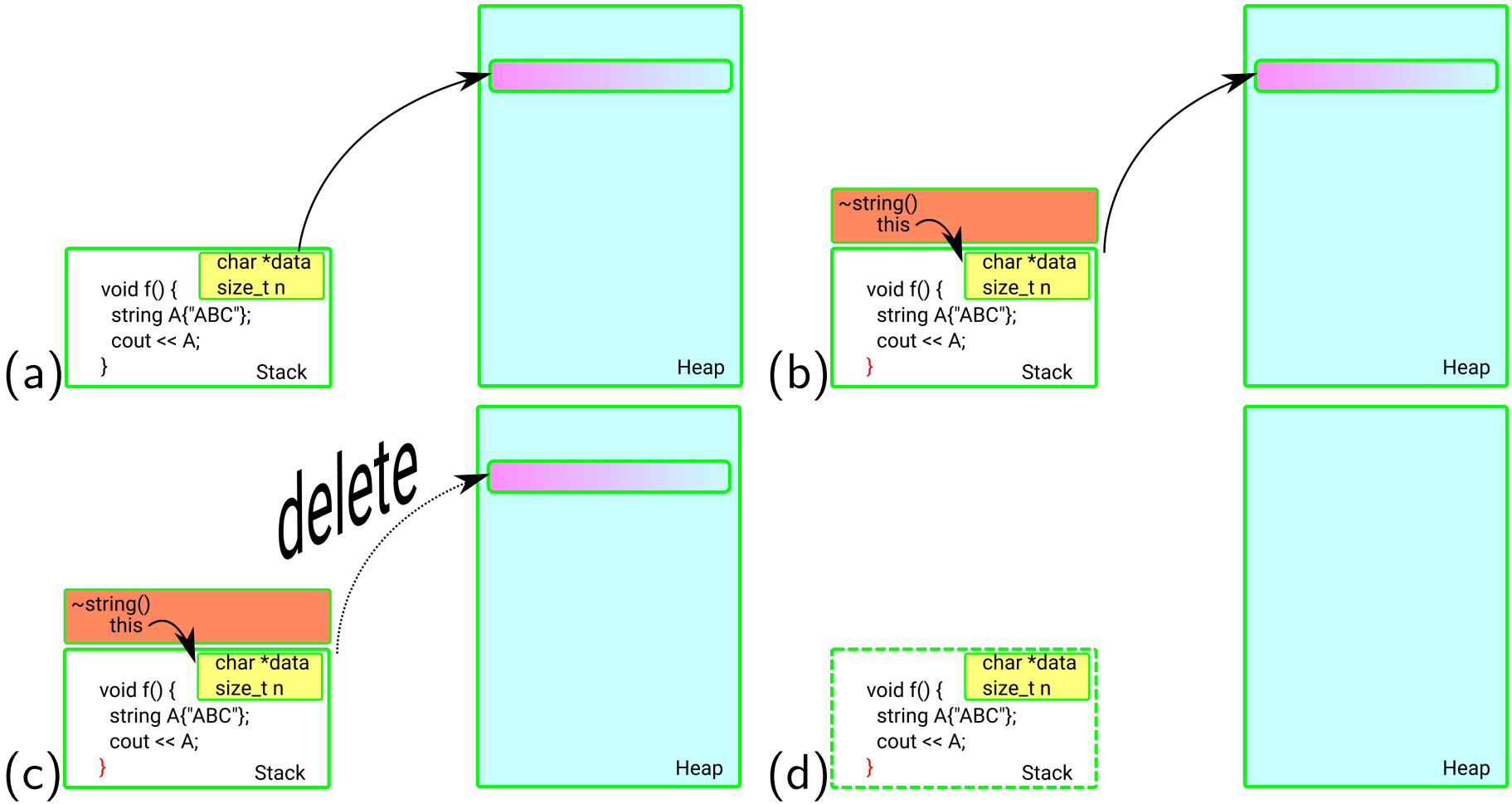
Resource handles and heap allocated data

Resource handles

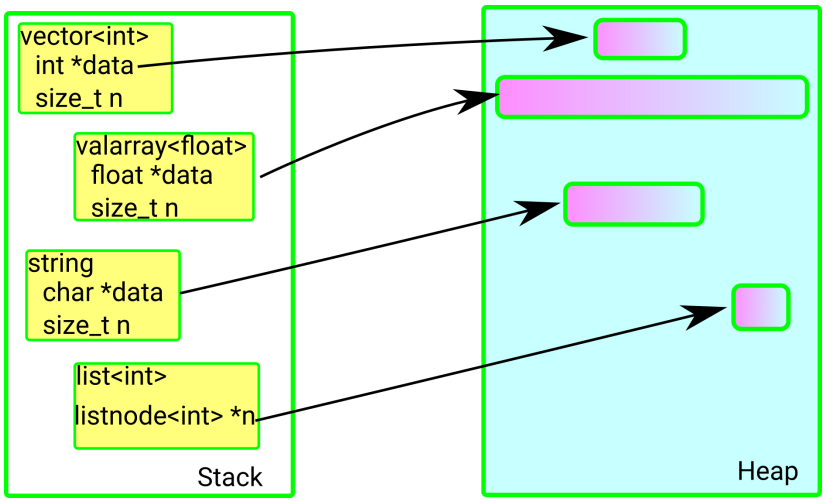
- Instead of bare heap allocation/deallocation, allocate in constructors or member functions (a)
- When the scope of the variable ends, the destructor is automatically called (b)
- Destructor should free any resources still in use (c)
- The variable can now expire (d)

The labels (a), (b), (c) and (d) refer to the figures in the following slide.

Resource handles

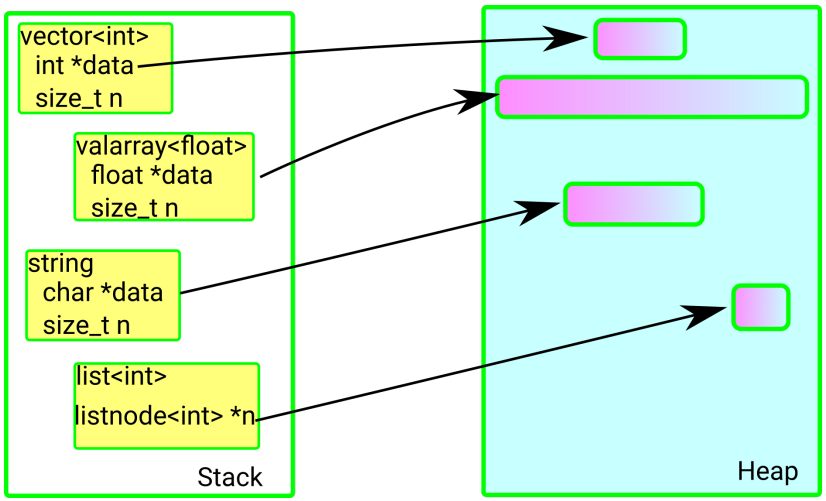


Resource handles



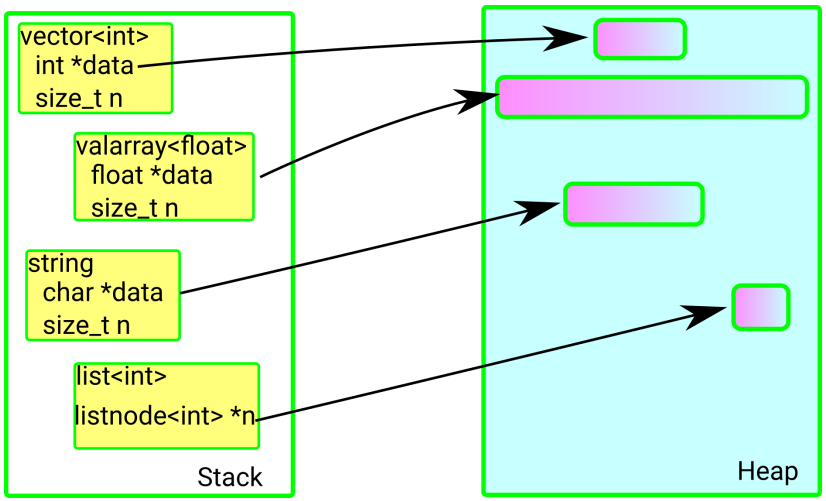
- STL containers (except `std::array`) are "resource" handles

Resource handles



- STL containers (except `std::array`) are "resource" handles
- Memory management is done through constructors, the destructor and member functions

Resource handles



- STL containers (except `std::array`) are "resource" handles
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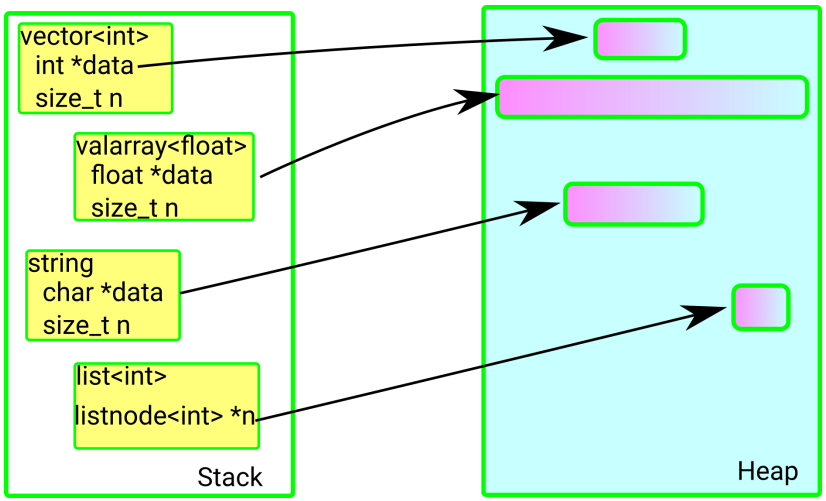
- No legitimate use of objects of the class should result in a memory leak

Resource handles



- STL containers (except `std::array`) are "resource" handles
- Memory management is done through constructors, the destructor and member functions

- No legitimate use of objects of the class should result in a memory leak
- Most data is on the heap. The objects on the stack are light-weight handles.

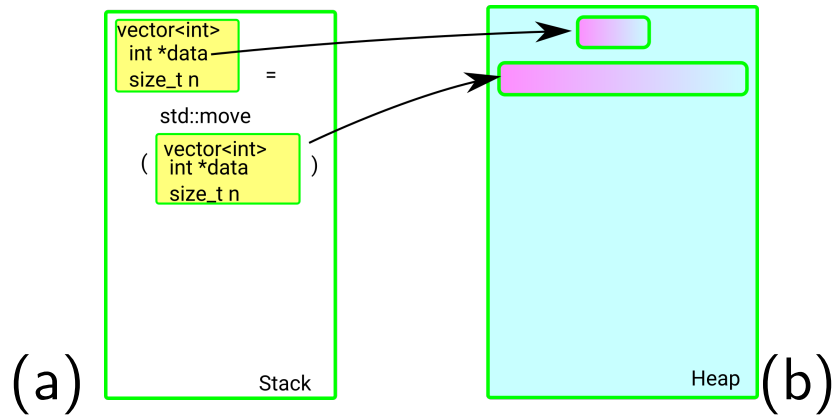
Resource handles

```
vector<int> A(32,0);
vector<double> B(64,0.);
vector<complex<double>> C(128);
vector<bool> D(256);
cout << sizeof(A) << "\n"
     << sizeof(B) << "\n"
     << sizeof(C) << "\n"
     << sizeof(C) << "\n";
```

Quiz

What will the program print ?

Resource handles

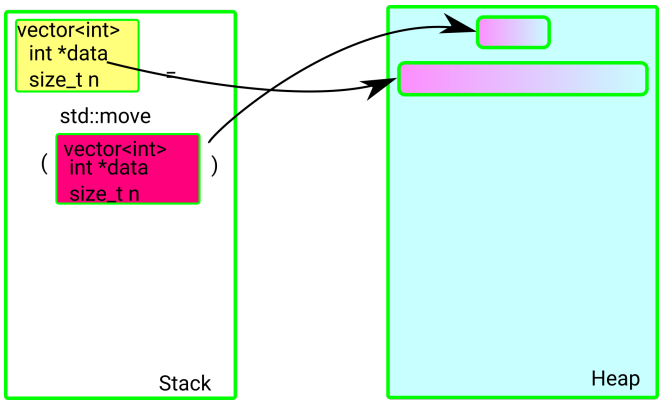


Move

- Can transfer ownership of the resources very cheaply

Resource handles

(a) (b)

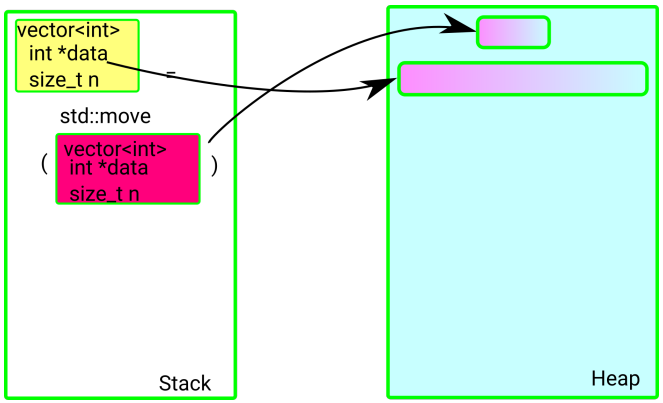


Move

- Can transfer ownership of the resources very cheaply
- Actual data on the heap need not be touched at all!

Resource handles

(a) (b)

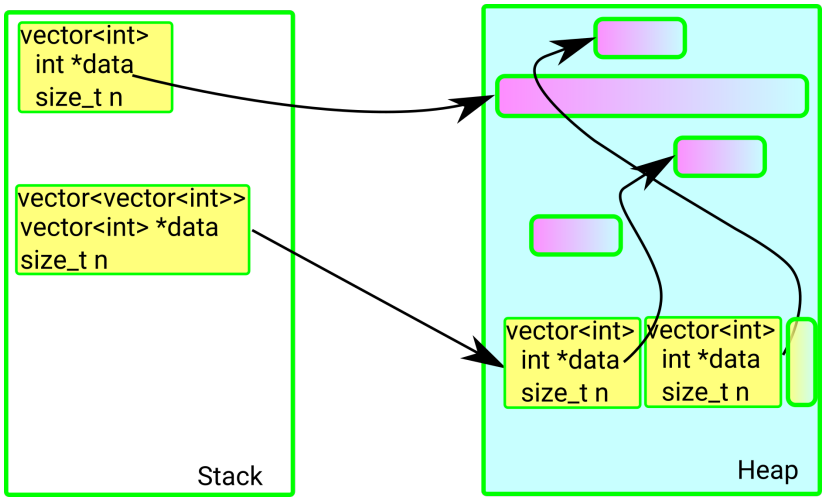


Move

- Can transfer ownership of the resources very cheaply
- Actual data on the heap need not be touched at all!
- Just some pointer re-assignments on the stack (a), (b)

Resource handles

```
vector<vector<int>> v(10,
                      vector<int>(10,0));
...
for (int i=0;i<10;++i) {
  for (int j=0;j<10;++j) {
    v[i][j]=i+j;
    //v.operator[](i).operator[](j);
    //(*(*(v.dat+i)).dat+j)
  }
}
```



- In C++, objects (instances of a class) can live on the stack or on the heap

Resource handles

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vector<vector<int>> v(10,
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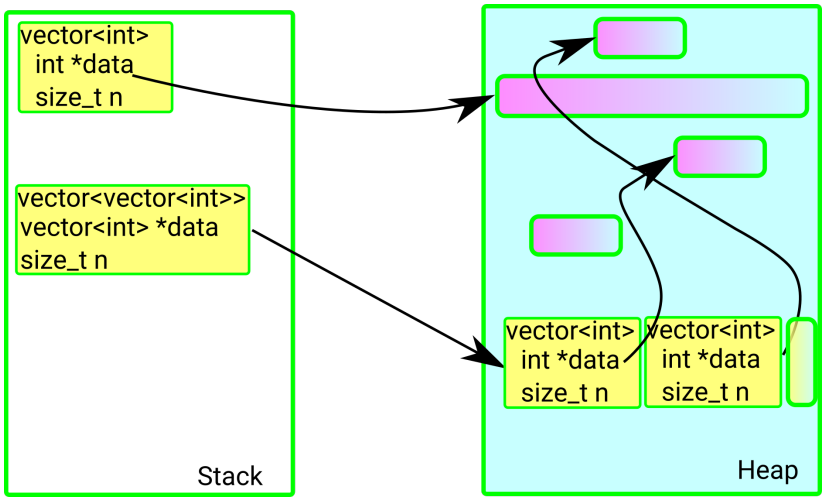
...
for (int i=0;i<10;++i) {
  for (int j=0;j<10;++j) {
    v[i][j]=i+j;
    //v.operator[](i).operator[](j);
    //(*(*(v.dat+i)).dat+j)
  }
}
```



- In C++, objects (instances of a class) can live on the stack or on the heap
- Putting resource handles like `vector<int>` on the heap, while allowed, incurs the cost of additional indirections

Resource handles

```
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                      vector<int>(10,0));
...
for (int i=0;i<10;++i) {
  for (int j=0;j<10;++j) {
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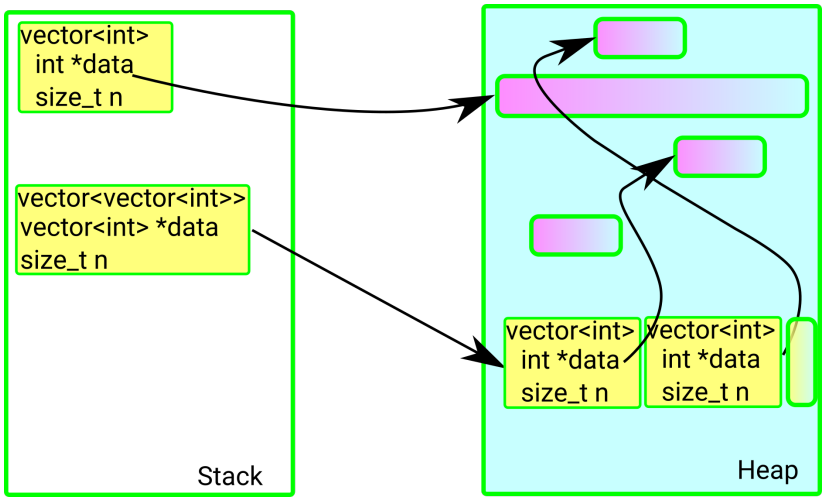
}
```



- In C++, objects (instances of a class) can live on the stack or on the heap
- Putting resource handles like `vector<int>` on the heap, while allowed, incurs the cost of additional indirections
- When possible, avoid cumbersome beasts like `vector<vector<int>>`

If you need your own 2D arrays, ...

```
template <typename T> class array2d {
  vector<T> v;
  size_t nc{0},nr{0};
public:
  T & operator()(size_t i, size_t j) {
    return v[i*nc+j];
  }
  // and a const version of the above
  template <typename U> struct row_t {
    vector<U> & orig;
    size_t offst, strd;
    explicit row_t(vector<U> &vv,
                   size_t i, size_t st) :
                   orig(vv), offst(i),
                   strd(st) {}
    U & operator[](size_t i) {
      return orig[offst+i*strd];
    }
  };
  row_t<T> operator[](size_t i) {
    return row_t(v,i*nc,1);
  }
};
```

- Use a wrapper class around an STL container, like `vector` or `valarray`
- Either overload the **`operator`**`()` to access a given row and column ...
- ... or use a helper class for rows to mimic 2D arrays in C

Example 4:

`examples/array2d` contains the template class shown here.

std::array

```
#include <iostream>
#include <array>

int main()
{
    std::array<double,10> A{{0.0,0.1,0.2,0.3,0.4,0.5,0.6,0.7,0.7,0.9}};
    std::cout << "Size of array on stack = "<<sizeof(A) <<"\n";
    std::cout << "size() = "<<A.size() <<"\n";
}
```

- Resembles other STL containers, but this is not just a handle.

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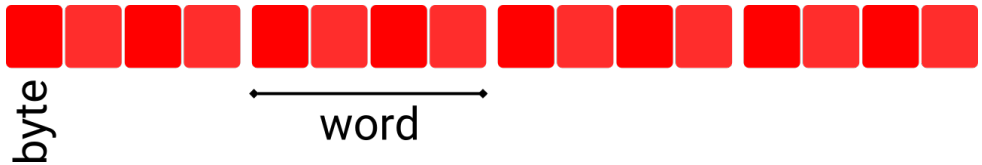
}
```

- Resembles other STL containers, but this is not just a handle.
- Does not need a data element to store the size, as the size is "part of the name" of the type!
- Moving an `std::array` has order N complexity, as each individual element needs to be moved. No pointer swapping trick can do the job for this.

Data alignment



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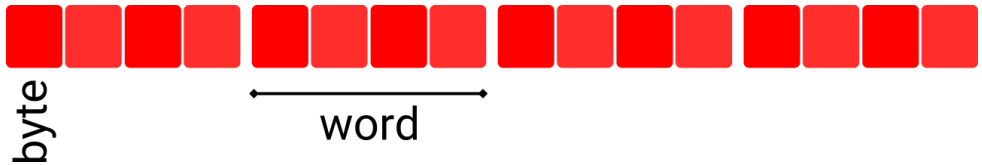
Data alignment



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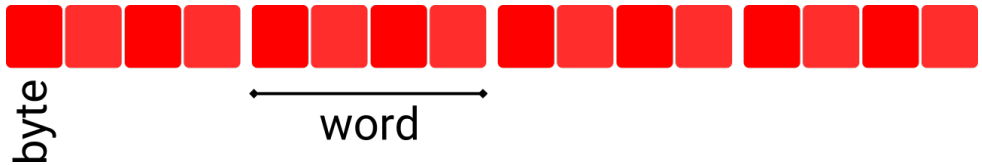

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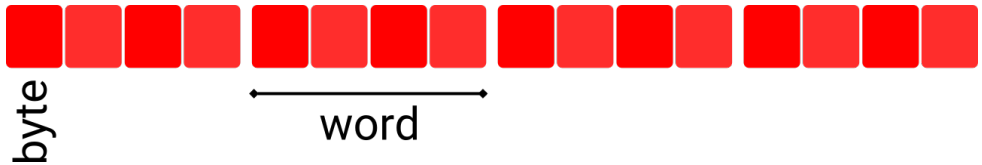

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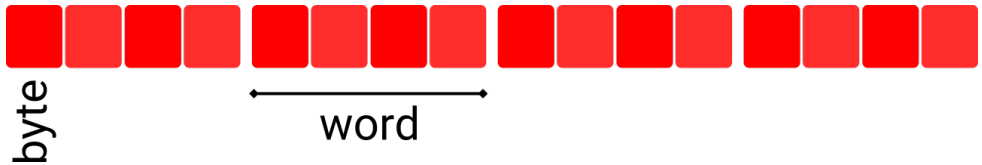

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- n-byte aligned address has $>= log_2(n)$ least significant zeros
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- If the size of a primitive type does not exceed the word size, access to aligned data of that type is also atomic

Data alignment

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- PowerPC throws a hardware exception, which may be handled by the OS. For unaligned 8 byte access, a 4,610% performance penalty has been discussed (http://www.ibm.com/developerworks/library/pa-dalign/)
- On other systems, crashes, data corruption, incorrect results are all possibilities

Data alignment

- Usually, primitive types are aligned by their "natural alignment": 4 byte **`int`** has 4 byte alignment, 8 byte double has alignment of 8 and so on
- A class has a natural alignment equal to the strictest requirement of its members
- The `alignof` operator can be used to query the alignment of a type
- The `alignas` keyword can be used to set a stricter alignment requirement

Example 5:

Verify the above using the example program `examples/align/alignof.cc`.

Data structure padding

```
class A {
  char c;
  double x;
  int d;
};
// Compiled as if it was ...
char c;
char pad[7];
double x;
int d;
char pad2[4]; // why is this here ?
// Overall alignment alignof(double)
// size of struct = 24
class B {
  double x;
  int d;
  char c;
};
// Compiled as if it was ...
double x;
int d;
char c;
char pad[3];
// Overall alignment alignof(double)
// size of struct = 16
```

- Alignment requirement of members can necessitate introduction of padding between members

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- Alignment requirement of members can necessitate introduction of padding between members
- Size of structures can therefore be bigger than the sum of sizes of their elements
- C++ rules do not allow the compiler to reorder elements for space
- Carefully choosing the declaration order of class members can save memory

alignas

```
alignas(64) double x[4]; // ok

alignas(64) vector<double>(4) a;
// Pointless.
// The above simply aligns the resource
// handle, not the data on the heap

alignas(64) array<double,4> A;
// This is fine, as std::array has
// real data in its struct

template <typename T, int vecsize>
struct alignas(vecsize) simd_t
{
  array<T,vecsize/sizeof(T)> data;
};
```

- The `alignas` keyword can specify alignment for variables
- Can be attached to a class declaration so that all objects of that type have a specified alignment
- Be mindful about what you are aligning when you use `alignas` for a resource handle like `vector` or `valarray`

Example 6:

The `examples/align/align0.cc` has a concept of a template class which creates a data array of the right size to fill the vector length irrespective of the input data type. It illustrates the use of `alignof` and `alignas`.

std::align

```
void* align(size_t alignment, size_t size, void*& ptr, size_t& space );
```

- Given a buffer, find a suitably aligned starting address inside it

std::align

```
void* align(size_t alignment, size_t size, void*& ptr, size_t& space );
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- `alignment` is the sought alignment of data. `ptr` is increased until it lands on an address with this alignment.

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void* align(size_t alignment, size_t size, void*& ptr, size_t& space );
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- Given a buffer, find a suitably aligned starting address inside it
- The starting value of `ptr` is used as the starting memory location
- The starting value of `space` is used as the remaining number of bytes in buffer
- `alignment` is the sought alignment of data. `ptr` is increased until it lands on an address with this alignment.
- `size` is the size of the object(s) intended for the aligned memory. If, after moving `ptr` we have less than `size` bytes left, the operation fails, and `nullptr` is returned

std::aligned_storage

```
template <size_t Length, size_t Alignment>
struct aligned_storage {
  using type=struct {alignas (Alignment) unsigned char data[Length]; };
  // Obs: This is the idea, not necessarily the real implementation!
};
template <size_t Length, size_t Alignment>
using aligned_storage_t = typename aligned_storage<Length, Alignment>::type;
```

- Raw uninitialized storage type for use by any type with size at most `Length` and alignment a divisor of `Alignment`

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```

- Raw uninitialized storage type for use by any type with size at most `Length` and alignment a divisor of `Alignment`
- Convenient alias `aligned_storage_t` available in C++14
- Used with "placement new" operator and explicit destructor calls to create/destroy objects of different types

The placement new operator

```
// Allocation and deallocation with new
double * d = new double[4];
delete [] d;

Protein * p=new Protein("nmrstruc.xml");
//
delete p;
```

```
// Usage of "placement new"
// There exists an uninitialized buffer
// on the stack or the heap.

Protein * p
  = new(buffer) Protein("nmrstruc.xml");
// Use existing location, but initialize
// with given constructor.
p->~Protein();
// Call destructor, but don't free.
```

- **new** : Obtain memory buffer and run a constructor on it.

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// Call destructor, but don't free.
```

- **`new`** : Obtain memory buffer and run a constructor on it.
- "Placement new" operator: We have a buffer, just run the constructor.
- Since placement **`new`** does not obtain memory itself, it should not be paired with a **`delete`** but rather an explicit destructor call at that pointer location

Example 7:

`examples/align/stdalign.cc` illustrates the use of `std::align` through a use defined allocator class, which can allocate memory from an internal buffer, through an allocate function which takes an alignment requirement as an argument. The original example is from `en.cppreference.com`, which I have modified slightly and commented with additional explanations.

Example 8:

`examples/align/aligned_storage.cc` illustrates the use of `std::aligned_storage`, `std::forward`, the placement **`new`** operator and explicit destructor calls. The original example is from `en.cppreference.com`, which I have modified slightly and commented with additional explanations. Please study the code, run it, understand the output and ask if you have any difficulties.

Cost of various abstractions

Reading assembly code

Exercise 2:

The website https://godbolt.org provides a great tool to quickly examine the assembly code corresponding to a code snippet. It is possible to choose different compilers, give compiler options ... Use it to quickly check the assembly code generated for simple functions. Compare different compilers. A few ideas on what to try are in the folder `examples/assembly`.

See also: CppCon 2016: Serge Guelton "C++ Costless Abstractions: the compiler view"

JÜLICH
FORSCHUNGSZENTRUM

Branching

pipeline

- Program execution flows through different units responsible for different work

- Instruction fetch
- Instruction decode
- Instruction execute
- Memory access
- Register write back

```
if (x+y>5) f();
else g();
```

- request mem x
- request mem y
- calc x+y
- calc res > 5
- ?

The "next instruction" depends on the outcome of an instruction.

Branch prediction

```
for (int i=0;i<N;++i) {
  if (p[i] > gen()) {
    b[i] = a[i]+c[i];
    ++fwd;
  } else {
    a[i] = b[i]+c[i];
    ++rev;
  }
}
nngb=0;
while (a) {
  dist[nngb++]=distf(a,i);
}
```

- For efficient execution, different units in the pipeline must be kept busy as much as possible

- When branches are encountered, the CPU simply guesses which way it will go, and fetches instructions accordingly
- If the guess is right, no pipeline stall
- If it is wrong, all operations done with that guess must be purged

Branch mis-prediction penalty

```
for (int i=0;i<N;++i) {
  if (p[i] > gen()) {
    a[i]=(b[i]>r0 && b[i] < r1
          && c[i]<b[i]);
  } else {
    a[i] = b[i]+c[i];
    ++rev;
  }
}
nngb=0;
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  dist[nngb++]=distf(a,i);
}
```

- If statements, switches, loops contain obvious branches
- The ternary operator `a = cond ? v1 : v2` is (not always!) a branch

- Not so obvious branches include boolean `||` and `&&` operators:

Branch mis-prediction penalty

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  - In a sequence of operations like `a || b || c || ...`, the operands are evaluated left to right until the first true value is obtained

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    ++rev;
  }
}
nngb=0;
while (a) {
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}
```

- If statements, switches, loops contain obvious branches
- The ternary operator `a = cond ? v1 : v2` is (not always!) a branch

- Not so obvious branches include boolean `||` and `&&` operators:
  - In a sequence of operations like `a || b || c || ...`, the operands are evaluated left to right until the first true value is obtained
  - In a sequence of operations like `a && b && c && ...`, the operands are evaluated left to right until the first false value is obtained

Not branches

```
 int f(int i)
{
    static const int a[4]={4,3,2,1};
    int ans=0;
    ans += (a[1]<i)?1:2;
    return ans;
}
```

```
0000000000000000 <_Z1fi>:
  cmp    edi,0x4
  setl   al
  movzx  eax,al
  inc    eax
  ret
```

- Conditional assignments are often reorganised as simple sequential instructions by compilers using assembly language tricks

```
0000000000000000 <_Z1fdPd>:
  subsd  xmm0,QWORD PTR [rdi]
  subsd  xmm0,QWORD PTR [rdi+0x8]
  subsd  xmm0,QWORD PTR [rdi+0x10]
  subsd  xmm0,QWORD PTR [rdi+0x18]
  ret
```

Not branches

```
double f(double x, double A[4])
{
    double a=x;
    for (int i=0;i<4;++i) a-=A[i];
    return a;
}
```

- Conditional assignments are often reorganised as simple sequential instructions by compilers using assembly language tricks
- Loops with small loop counts may be automatically unrolled at compile time leaving simple linear code

```
0000000000000000 <_Z1fdPd>:
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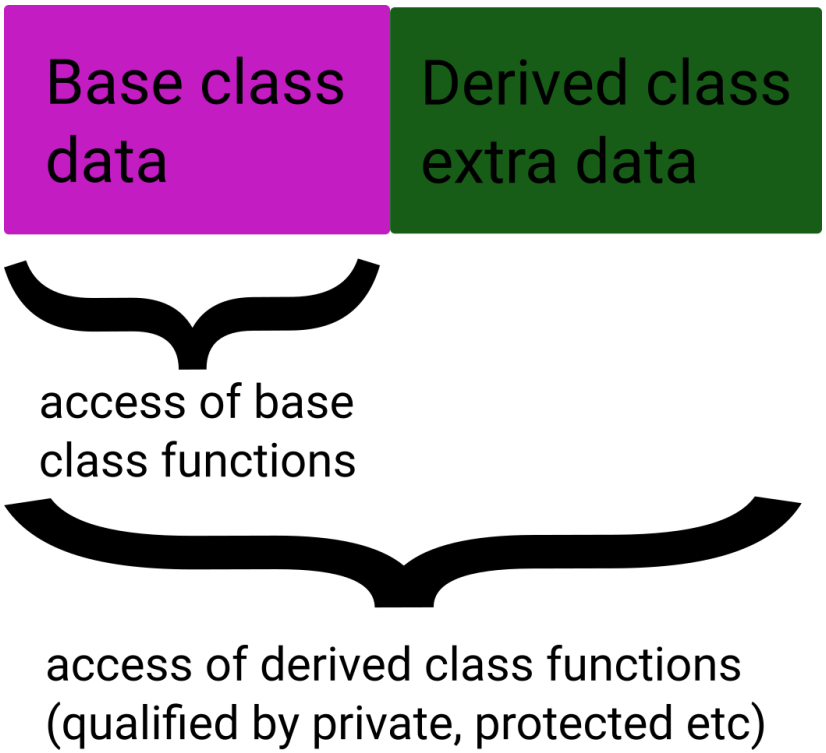
  subsd   xmm0,QWORD PTR [rdi+0x8]
  subsd   xmm0,QWORD PTR [rdi+0x10]
  subsd   xmm0,QWORD PTR [rdi+0x18]
  ret
```

Example 9:

Branch prediction effectiveness varies a lot between CPUs. Using the example program `examples/branch_prediction.cc`, compare the Sandy bridge series of processors on your workstations with the Haswell processors on JURECA. The program partitions an array of integers into 3 ranges. Running it with a command line argument (value ignored) causes it to first sort the array and then perform the same partitioning actions. In the sorted array, the branches are easier to predict. What do you observe ?

Class hierarchies

Inheritance



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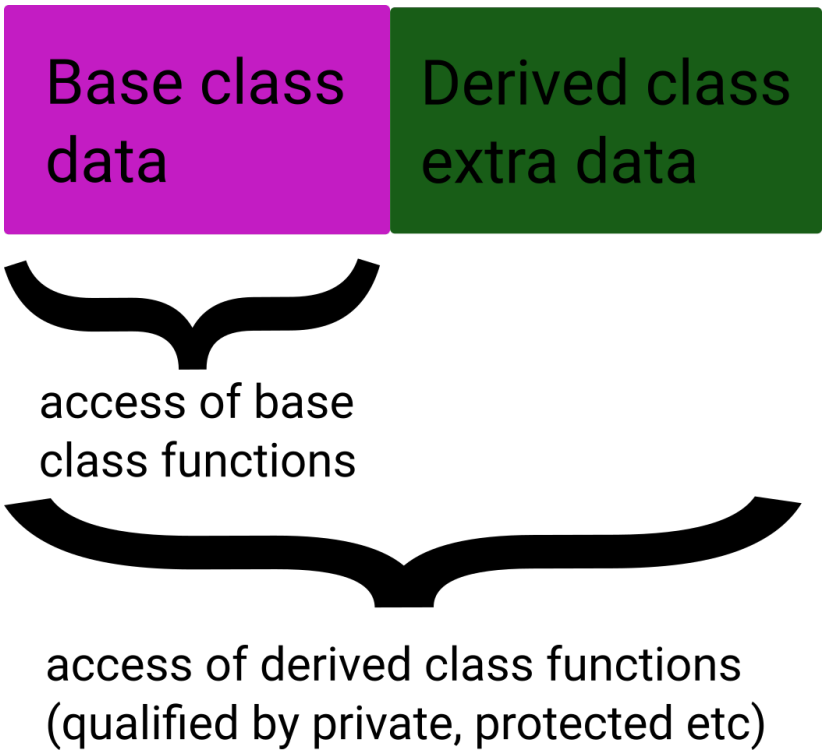

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- The base class functions, if invoked, will see a base class object

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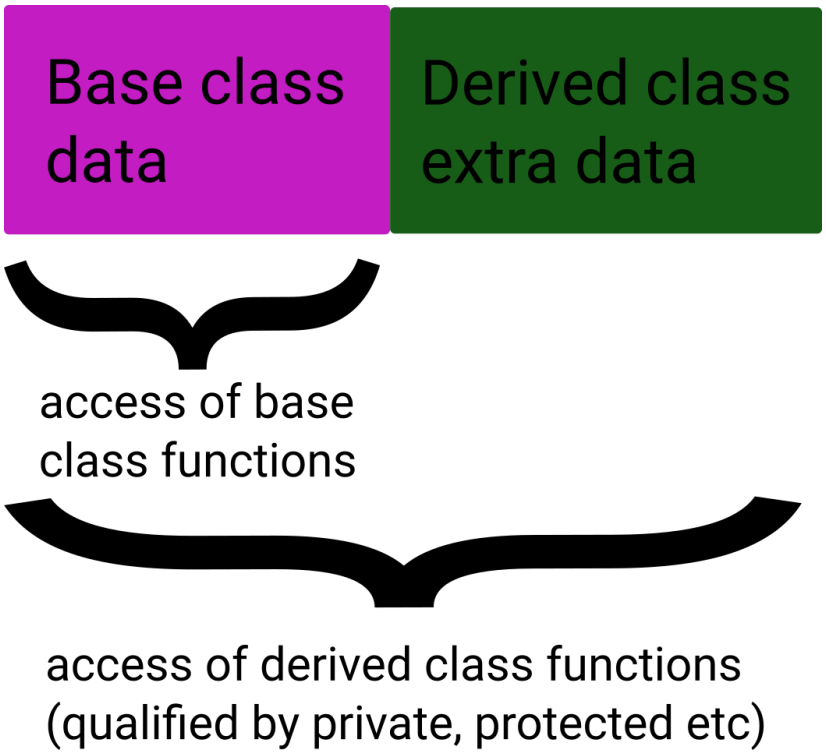
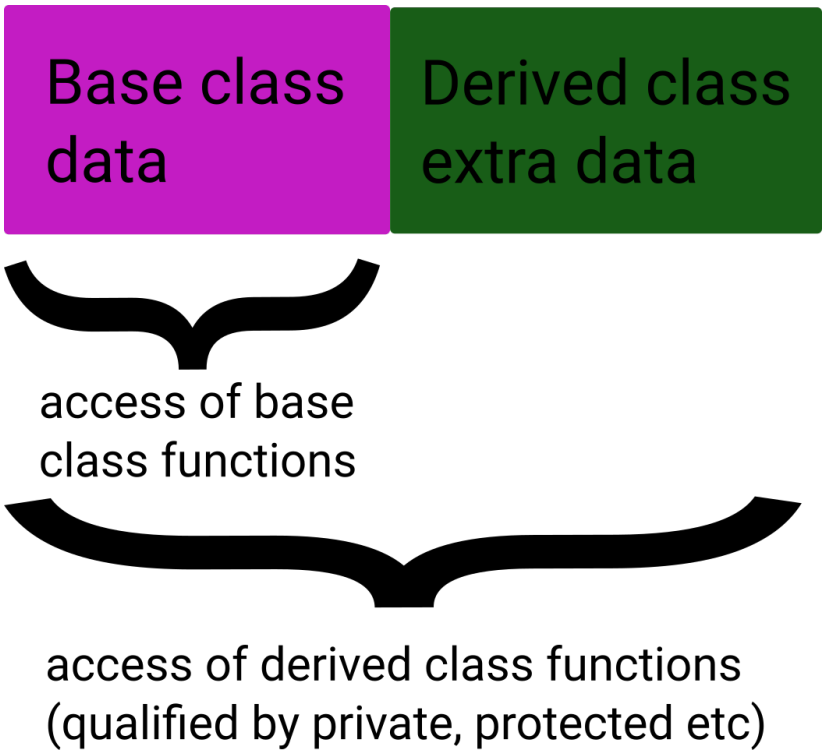


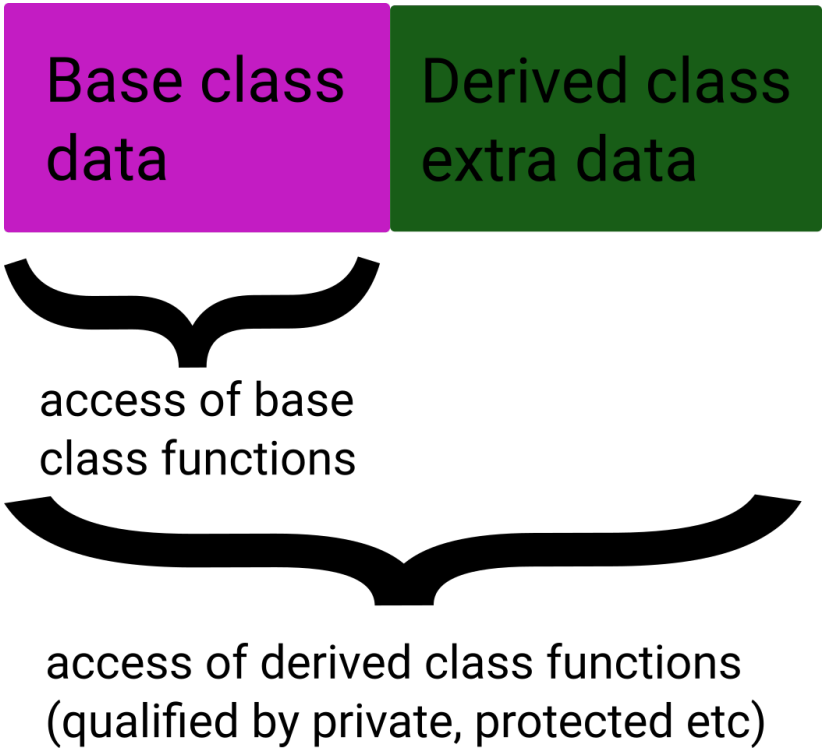
- Inheriting class may add more data, but it retains all the data of the base
- The base class functions, if invoked, will see a base class object
- The derived class object *is a* base class object, but with additional properties

Inheritance



- A pointer to a derived class always points to an address which also contains a valid base class object.

Inheritance



- A pointer to a derived class always points to an address which also contains a valid base class object.
- `baseptr=derivedptr` is called "upcasting". Always allowed.

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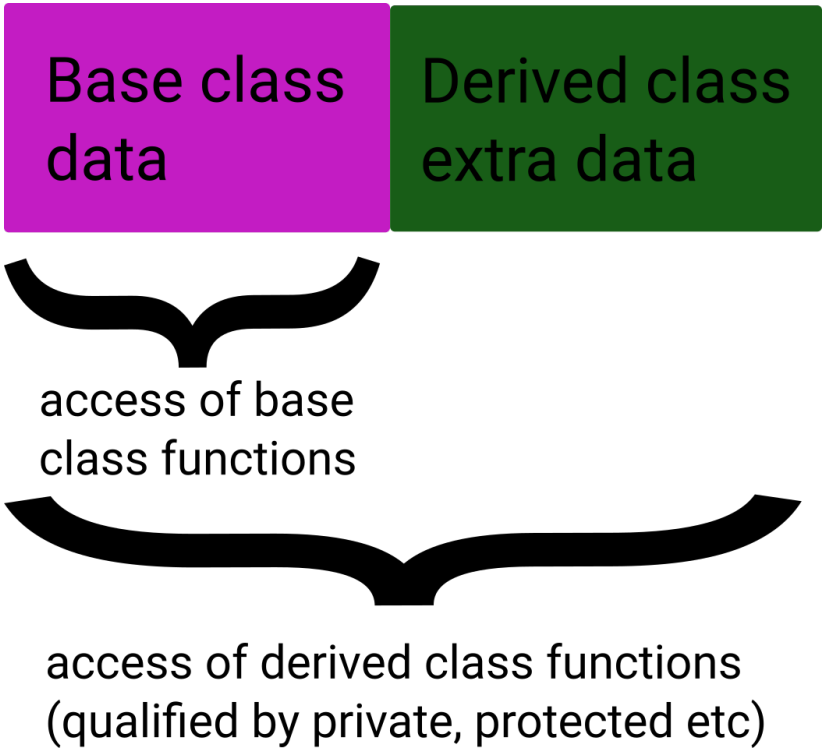
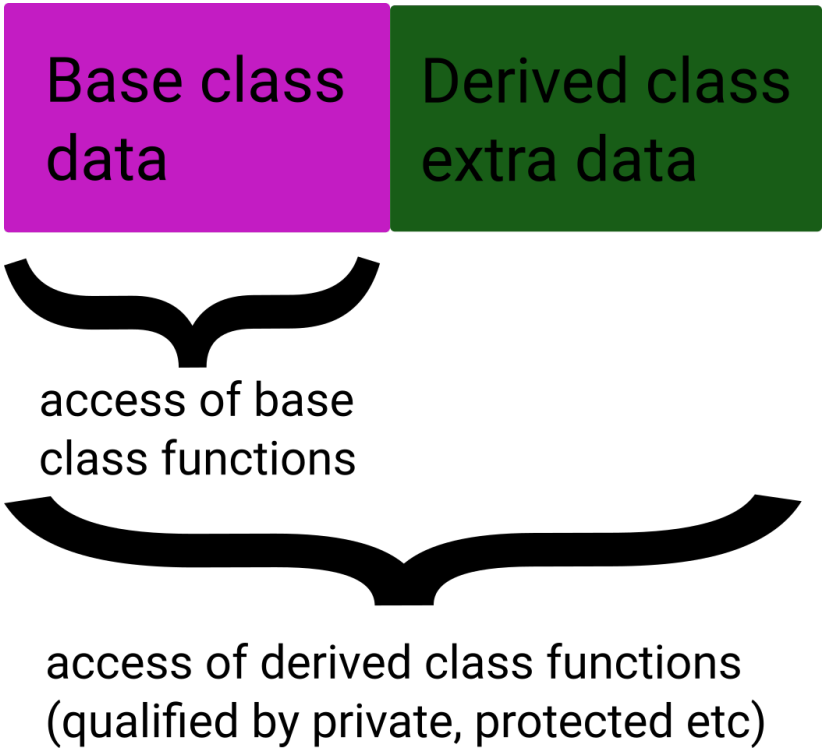


- A pointer to a derived class always points to an address which also contains a valid base class object.
- `baseptr=derivedptr` is called "upcasting". Always allowed.
- Implicit downcasting is not allowed. Explicit downcasting is possible with **`static_cast`** and **`dynamic_cast`**

Inheritance




```
class Base {
public:
  void f(){std::cout<<"Base::f()\n";}
protected:
  int i{4};
};
class Derived : public Base {
  int k{0};
public:
  void g(){std::cout<<"Derived::g()\n";}
};
int main()
{
  Derived b;
  Base *ptr=&b;
  ptr->g(); // Error!
  static_cast<Derived *>(ptr)->g(); //OK
}
```

Class inheritance with virtual functions

```
int main()
{
  darray<Shape *> shape;
  shape.push_back(new Circle(0.5, Point(3,7)));
  shape.push_back(new Triangle(Point(1,2),Point(3,3),Point(2.5,0)));
...
  for (size_t i=0;i<shape.size();++i) {
    std::cout<<shape[i]->area()<<'\n';
  }
}
```

- A pointer to a base class is allowed to point to an object of a derived class

Class inheritance with virtual functions

```
int main()
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}
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- A pointer to a base class is allowed to point to an object of a derived class
- Here, `shape[0]->area()` will call `Circle::area()`, `shape[1]->area()` will call `Triangle::area()`

Class inheritance with virtual functions

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  shape.push_back(new Circle(0.5, Point(3,7)));
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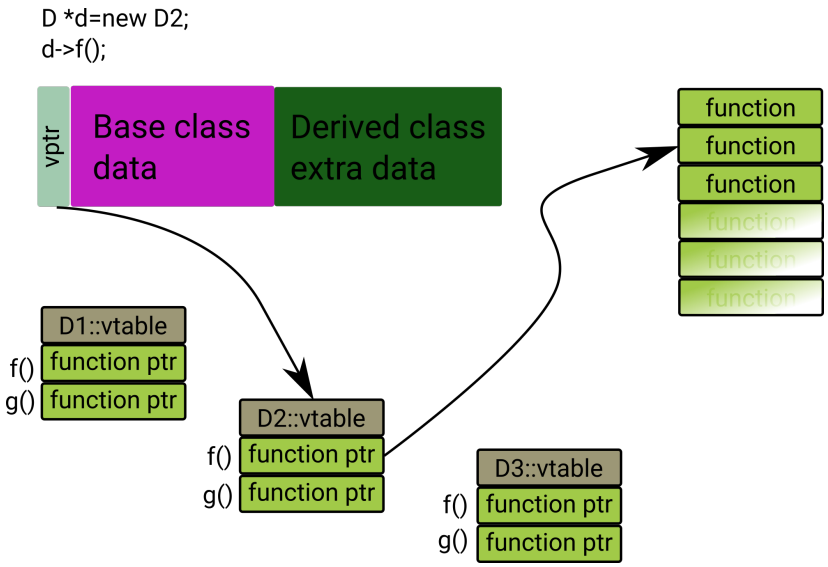
...
  for (size_t i=0;i<shape.size();++i) {
    std::cout<<shape[i]->area()<<'\n';
  }
}
```

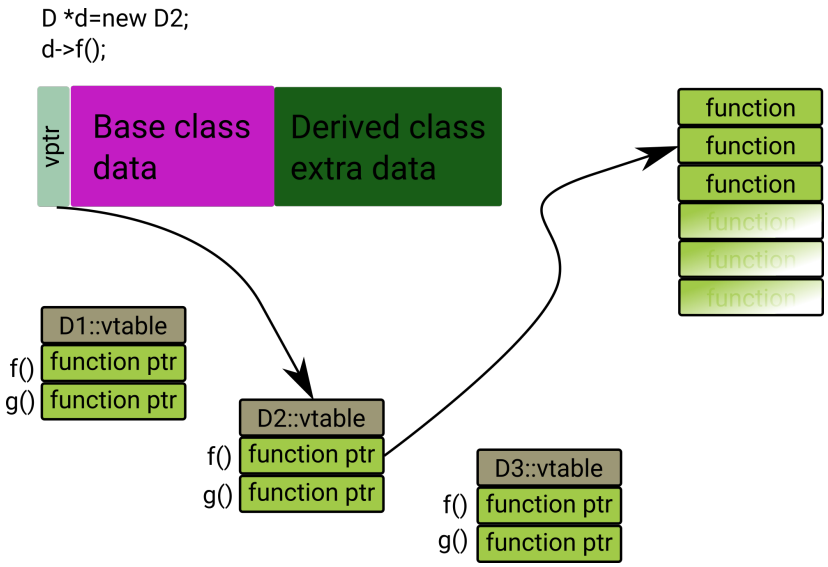
- A pointer to a base class is allowed to point to an object of a derived class
- Here, `shape[0]->area()` will call `Circle::area()`, `shape[1]->area()` will call `Triangle::area()`
- But, how does it work ?

Calling virtual functions: how it works



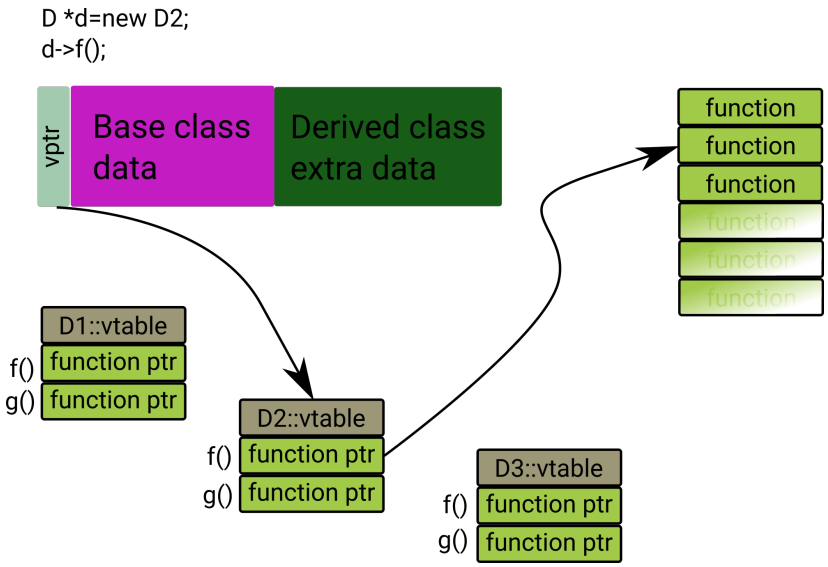
- For classes with virtual functions, the compiler inserts an invisible pointer member to the data and additional book keeping code

Calling virtual functions: how it works



- For classes with virtual functions, the compiler inserts an invisible pointer member to the data and additional book keeping code
- There is a table of virtual functions for each derived class, with entries pointing to function code somewhere

Calling virtual functions: how it works



- For classes with virtual functions, the compiler inserts an invisible pointer member to the data and additional book keeping code
- There is a table of virtual functions for each derived class, with entries pointing to function code somewhere
- The `vptr` pointer points to the *vtable* of that particular class

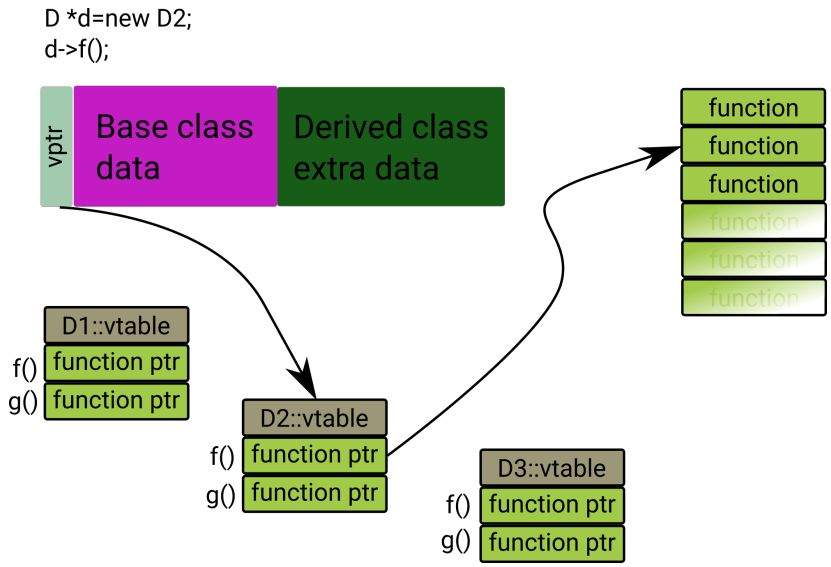
vptr

Example 10:

The program `examples/vptr.cc` gives you a tiny class with two **`double`** data members. The `main` function simply creates an object of this kind and prints its size. It prints 16 (bytes) as expected. Uncomment a line containing a virtual destructor function for this class, and recompile and re-run. It will now print 24 as the size on a typical 64 bit machine. Compiling with `g++ -O0 -g3 --no-`**`inline`** and running it in the debugger, you can see the layout of the data structure in memory, and verify that the extra data member is indeed a pointer to a *vtable* for the class.

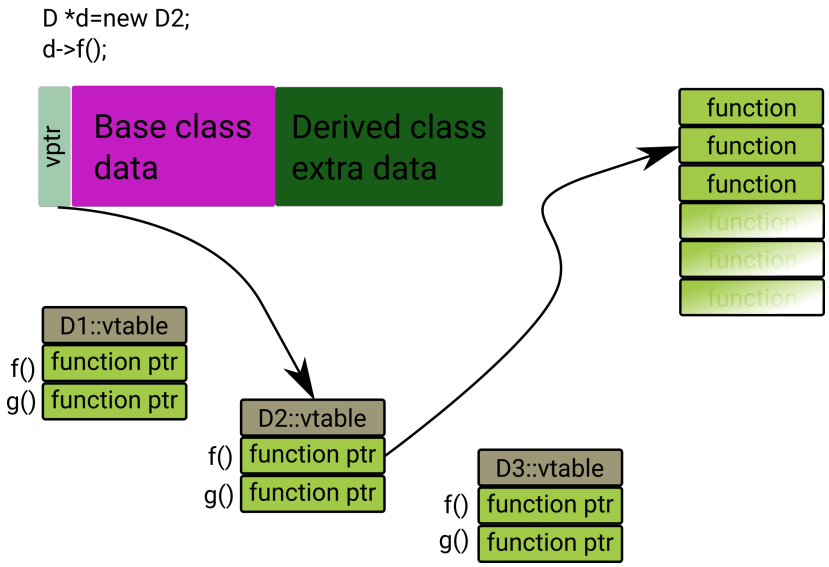
Calling virtual functions: how it works

- Virtual function call proceeds by first finding the right *vtable*, then the correct entry for the called function, dereferencing that function pointer and then executing the correct function body



Calling virtual functions: how it works

- Virtual function call proceeds by first finding the right *vtable*, then the correct entry for the called function, dereferencing that function pointer and then executing the correct function body
- For HPC applications, use of virtual functions in hot sections will hurt performance



Calling virtual functions: how it works

- Virtual function call proceeds by first finding the right *vtable*, then the correct entry for the called function, dereferencing that function pointer and then executing the correct function body
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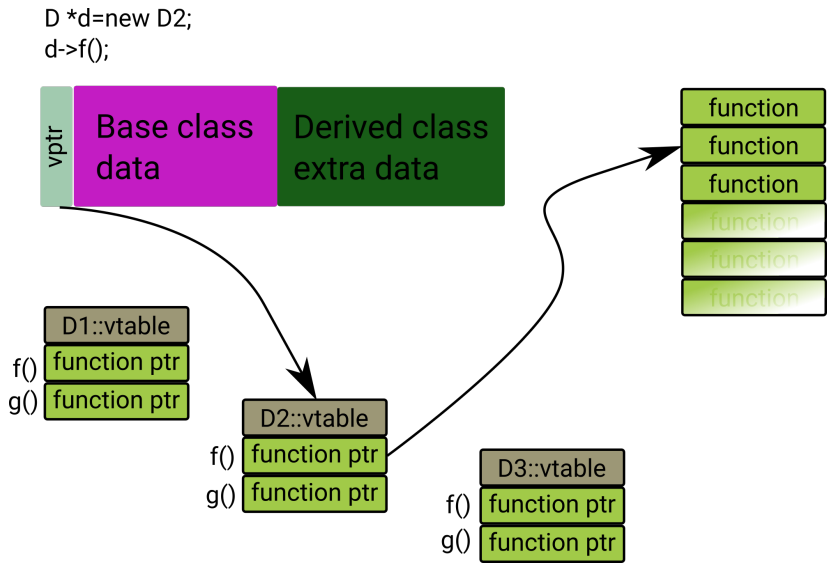

- Often, the polymorphic behaviour sought after using virtual functions can be implemented with CRTP without the virtual function overhead

Polymorphism without virtual functions

Tag dispatching

```
struct property1 {};
struct property2 {};
template <typename T>
void do_something(T && t, property1)
{
  std::cout << "Function objects with property1\n";
}
template <typename T>
void do_something(T && t, property2) {...}
//...
template <typename T>
void do_something(T t)
{
    do_something(t, typename T::tag{});
}
```

```
class Bird {
public:
  using tag = typename
        property1;
};
class SparseMatrix {
public:
  using tag = typename
        property2;
};
//...
Bird b;
do_something(b);
SparseMatrix m;
do_something(m);
```

- Logically similar operations on different types, where the operations depend on certain properties of the types

Tag dispatching

```
struct property1 {};
struct property2 {};
template <typename T>
void do_something(T && t, property1)
{
  std::cout << "Function objects with property1\n";
}
template <typename T>
void do_something(T && t, property2) {...}
//...
template <typename T>
void do_something(T t)
{
    do_something(t, typename T::tag{});
}
```

```
class Bird {
public:
  using tag = typename
        property1;
};
class SparseMatrix {
public:
  using tag = typename
        property2;
};
//...
Bird b;
do_something(b);
SparseMatrix m;
do_something(m);
```

- Logically similar operations on different types, where the operations depend on certain properties of the types
- "Dispatch" functions to guide the compiler to a suitable implementation based on a "tag" in the incomming type

SFINAE : Substitution Failure is not an Error

```
// Examples/sfinae0.cc
template <typename V>
void f(const V &v,
       typename V::iterator * jt=0)
{
  std::cout << "Container overload\n";
  for (auto x : v) std::cout <<  x <<" ";
  std::cout << "\n";
}

void f(...)
{
  std::cout << "Catch all overload\n";
}

int main()
{
  std::list<double> L
       {0.1,0.2,0.3,0.4,0.5,0.6};
  int A[4]{4,3,2,1};
  f(A);
  f(L);
}
```

- Overload resolution of templates

SFINAE : Substitution Failure is not an Error

```
// Examples/sfinae0.cc
template <typename V>
void f(const V &v,
       typename V::iterator * jt=0)
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  f(L);
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```

- Overload resolution of templates
- If substitution fails, overload discarded

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  f(A);
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- Overload resolution of templates
- If substitution fails, overload discarded
- All parameters, expressions and the return type in declarations

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void f(const V &v,
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  std::list<double> L
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  int A[4]{4,3,2,1};
  f(A);
  f(L);
}
```

- Overload resolution of templates
- If substitution fails, overload discarded
- All parameters, expressions and the return type in declarations
- Substitution failure : ill-formed type or expression when a substitution is made

SFINAE : Substitution Failure is not an Error

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       {0.1,0.2,0.3,0.4,0.5,0.6};
  int A[4]{4,3,2,1};
  f(A);
  f(L);
}
```

- Overload resolution of templates
- If substitution fails, overload discarded
- All parameters, expressions and the return type in declarations
- Substitution failure : ill-formed type or expression when a substitution is made
- Not in function body!

enable_if

```
template <bool B, class T>
struct enable_if;
template <class T>
struct enable_if<true, T> {
  using type=T
};
template <bool B, class T=void>
using enable_if_t=typename
                enable_if<B,T>::type;

template <typename T>
enable_if_t<is_integral<T>::value, T>
Power(T x, T y) {
  // Implementation suitable for
  // integral number parameters
}
template <typename T>
enable_if_t<is_floating_point<T>::value,
            T>
Power(T x, T y) {
  // Implementation suitable for
  // floating point parameters
}
```

- Only if the first parameter is true, the structure `enable_if` has a member type called `type` set to the second template parameter
- Using the `type` member of an `enable_if` struct in a declaration will lead to an ill-formed expression when the condition parameter is false. That version of the function will then be ignored

Example 11:

The tag dispatching technique is demonstrated in `examples/tag_dispatch.cc`.

Example 12:

`examples/sfinae0.cc` is a simple syntax illustration for SFINAE.

Example 13:

`examples/enableif0.cc` shows one use of `std::enable_if`. The parameter list of the two variants of the template function `f` are identical, and they are "templates", where the place holder typename `T` can take arbitrary values. Yet, we can create two versions of the function and have the compiler choose one or the other depending on the properties of the input type.

Choosing algorithm based on API

```
// C++17
template <class C> size_t algo(C && x)
{
  if constexpr (hasAPI<C>) {
    x.helper();
    return x.calculateFast();
  } else {
    return x.calculate();
  }
}
```

- We want to write a general algorithm for an operation
- In case the function argument has a certain member function, we have a neat and quick solution
- Otherwise, we have a fallback solution

Choosing algorithm based on API

```
template <typename T> struct hasAPI_t {
  using basetype =
    typename remove_reference<T>::type;
  template <class C>
  static constexpr auto test(C * x) ->
  decltype(x->calculateFast(),
           x->helper(),
           bool{})
  {
    return true;
  }
  static constexpr bool test(...) {
    return false;
  }
  static constexpr auto value =
   test(static_cast<basetype*>(nullptr));
};
```

- The "template function" `hasAPI_t` has a member `value` initialized via a **`constexpr`** function, which passes information about the templated type to the `test` function

Choosing algorithm based on API

```
template <typename T> struct hasAPI_t {
  using basetype =
    typename remove_reference<T>::type;
  template <class C>
  static constexpr auto test(C * x) ->
  decltype(x->calculateFast(),
           x->helper(),
           bool{})
  {
    return true;
  }
  static constexpr bool test(...) {
    return false;
  }
  static constexpr auto value =
   test(static_cast<basetype*>(nullptr));
};
```

- The "template function" `hasAPI_t` has a member `value` initialized via a **`constexpr`** function, which passes information about the templated type to the `test` function
- Two variants of the test function exist, one always returning false, to cover the "everything else" case

Choosing algorithm based on API

```
template <typename T> struct hasAPI_t {
  using basetype =
    typename remove_reference<T>::type;
  template <class C>
  static constexpr auto test(C * x) ->
  decltype(x->calculateFast(),
           x->helper(),
           bool{})
  {
    return true;
  }
  static constexpr bool test(...) {
    return false;
  }
  static constexpr auto value =
   test(static_cast<basetype*>(nullptr));
};
```

- The positive version of the `test` function defines its return type using `decltype`, but applying it to a comma separated list of necessary API expressions

Choosing algorithm based on API

```
template <typename T> struct hasAPI_t {
  using basetype =
    typename remove_reference<T>::type;
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  static constexpr auto test(C * x) ->
  decltype(x->calculateFast(),
           x->helper(),
           bool{})
  {
    return true;
  }
  static constexpr bool test(...) {
    return false;
  }
  static constexpr auto value =
   test(static_cast<basetype*>(nullptr));
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```

- The positive version of the `test` function defines its return type using `decltype`, but applying it to a comma separated list of necessary API expressions
- A comma separated list of expressions evaluates to the last value, but each value in the list is checked for syntax

Choosing algorithm based on API

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template <typename T> struct hasAPI_t {
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  static constexpr auto test(C * x) ->
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  static constexpr bool test(...) {
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};
```

- The positive version of the `test` function defines its return type using `decltype`, but applying it to a comma separated list of necessary API expressions
- A comma separated list of expressions evaluates to the last value, but each value in the list is checked for syntax
- If the type of the argument does not have the member functions, the return type of the function can not be determined, and the overload is rejected

Choosing algorithm based on API

```
template <typename T> constexpr bool hasAPI = hasAPI_t<T>::value;
template <class C> std::enable_if_t< hasAPI<C>, size_t > algo(C && x)
{
    x.helper();
    return x.calculateFast();
}
template <class C> std::enable_if_t< !hasAPI<C>, size_t > algo(C && x)
{
    return x.calculate();
}
```

- What remains, is to make a nice wrapper template variable so that we can say `hasAPI<T>`, instead of `hasAPI_t<T>::value` when we need it.

Choosing algorithm based on API

```
template <typename T> constexpr bool hasAPI = hasAPI_t<T>::value;
template <class C> std::enable_if_t< hasAPI<C>, size_t > algo(C && x)
{
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}
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{
    return x.calculate();
}
```

- What remains, is to make a nice wrapper template variable so that we can say `hasAPI<T>`, instead of `hasAPI_t<T>::value` when we need it.
- The dispatch functions are written using `enable_if_t`, so that we pick the `calculateFast` function over `calculate`, if it is available

Choosing algorithm based on API

```
int main()
{
    Machinery obj;
    auto res = algo(obj);
    std::cout << "Result = " << res << "\n";
}
```

- Users of our great algorithm can simply call our `algo()` in their code

Choosing algorithm based on API

```
int main()
{
    Machinery obj;
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    std::cout << "Result = " << res << "\n";
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- Users of our great algorithm can simply call our `algo()` in their code
- If they have a `calculate` function, everything will work.

Choosing algorithm based on API

```
int main()
{
    Machinery obj;
    auto res = algo(obj);
    std::cout << "Result = " << res << "\n";
}
```

- Users of our great algorithm can simply call our `algo()` in their code
- If they have a `calculate` function, everything will work.
- If they then go on to implement `calculateFast` in their `Machinery` class, without any changes at the call site, or in the `algo` function, the compiler will make sure that we are using the (hopefully) better, `calculateFast` function

Example 14:

The program `examples/shim1.cc` is an interesting application of SFINAE, where we determine whether a template argument passed to a template function is a type which has a member function called `size()`. Modify to detect another member function!

Example 15:

The folder `examples/apishimming` contains the example `hasAPI` template function used in this section, with an application that uses it. By freeing the commented implementation of `calculateFast`, and recompiling, you will see that the call to `algo` automatically switches to use `calculateFast`.

Curiously Recurring Template Pattern

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- You need types A and B which have some properties in common, which can be calculated using similar data

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- There are a few polymorphic functions, but conceptually A and B are so different that you don't expect to store them in a single pointer container

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- There are a few polymorphic functions, but conceptually A and B are so different that you don't expect to store them in a single pointer container
- The penalty of using virtual functions seems to matter

Curiously Recurring Template Pattern

- You need types A and B which have some properties in common, which can be calculated using similar data
- There are a few polymorphic functions, but conceptually A and B are so different that you don't expect to store them in a single pointer container
- The penalty of using virtual functions seems to matter
- Option 1: implement as totally different classes, just copy and paste the common functions
- Option 2: try the CRTP

Curiously Recurring Template Pattern

```
template <class D> struct Named {
  inline string get_name() const {
    // polymorphic function, simply
    // redirect to the class D given
    // as a template parameter. Wont compile
    // if D does not inherit from this class
    return static_cast<D const *>(this)
                ->get_name_impl();
  }
  inline int version() const {
    // Non-polymorphic "common" function
    return 42;
  }
};
struct Acetyl : public Named<Acetyl> {
  inline string get_name_impl() const {
    return "Acetyl";
  }
};
struct Car : public Named<Car> {
  inline string get_name_impl() const {
    return get_brand()+get_model()+
        get_year();
  }
};
```

```
int main()
{
  Acetyl a;
  Car b;
  cout << "get_name on a returns : "
       << a.get_name() << '\n';
  cout << "get_name on b returns : "
       << b.get_name() << '\n';
  cout << "Their versions are "
       << a.version()<< " and "
       << b.version()<<'\n';
}
```

CRTP

- Polymorphism without virtual functions
- Faster in many cases

Expression Templates

Expression Templates

```
template <typename T>
class vec {
  std::vector<T> dat;
public:
  vec(size_t n) : dat(n) {}
  T operator[](size_t i) const {
    return dat[i];
  }
  T & operator[](size_t i) {
    return dat[i];
  }
  size_t size() const{return dat.size();}
};
template <typename T>
vec<T> operator+(const vec<T> & v1,
                 const vec<T> & v2)
{
  assert(v1.size()==v2.size());
  auto ans=v1;
  for (size_t i=0;i<ans.size();++i)
    ans[i]+=v2[i];
  return ans;
}
```

```
vec<double> W(N), X(N), Y(N), Z(N);
//..
W = a*X + 2*a*Y + 3*a*Z;
```

- Naive implementation which elegantly expresses our intent

Expression Templates

```
template <typename T>
class vec {
  std::vector<T> dat;
public:
  vec(size_t n) : dat(n) {}
  T operator[](size_t i) const {
    return dat[i];
  }
  T & operator[](size_t i) {
    return dat[i];
  }
  size_t size() const{return dat.size();}
};
template <typename T>
vec<T> operator+(const vec<T> & v1,
                 const vec<T> & v2)
{
  assert(v1.size()==v2.size());
  auto ans=v1;
  for (size_t i=0;i<ans.size();++i)
    ans[i]+=v2[i];
  return ans;
}
```

```
vec<double> W(N), X(N), Y(N), Z(N);
//..
W = a*X + 2*a*Y + 3*a*Z;
```

- Naive implementation which elegantly expresses our intent
- Each multiplication and addition creates a temporary and does a loop over elements

Expression Templates

```
template <typename T>
class vec {
  std::vector<T> dat;
public:
  vec(size_t n) : dat(n) {}
  T operator[](size_t i) const {
    return dat[i];
  }
  T & operator[](size_t i) {
    return dat[i];
  }
  size_t size() const{return dat.size();}
};
template <typename T>
vec<T> operator+(const vec<T> & v1,
                 const vec<T> & v2)
{
  assert(v1.size()==v2.size());
  auto ans=v1;
  for (size_t i=0;i<ans.size();++i)
    ans[i]+=v2[i];
  return ans;
}
```

```
vec<double> W(N), X(N), Y(N), Z(N);
//..
W = a*X + 2*a*Y + 3*a*Z;
```

- Naive implementation which elegantly expresses our intent
- Each multiplication and addition creates a temporary and does a loop over elements
- Poor performance

Expression templates

If only we had a special class ...

- ... which stored references to `X`, `Y` and `Z`

Expression templates

If only we had a special class ...

- ... which stored references to `X`, `Y` and `Z`
- and had an **`operator`**`[]` which returns

```
a*X[i]+2*a*Y[i]+3*a*Z[i]
```

Expression templates

If only we had a special class ...

- ... which stored references to `X`, `Y` and `Z`
- and had an **`operator[]`** which returns `a*X[i]+2*a*Y[i]+3*a*Z[i]`
- We could equip our `vec` class with a special assignment operator taking this special class as the right hand side

```
template <typename T>
class vec {
  template <class XPR>
  vec & operator=(const XPR & r)
  {
    for (size_t i=0;i<size();++i) {
      dat[i]=r[i]; // and r[i] returns a*X[i]+2*a*Y[i]+3*a*Z[i]
    } // One single loop, no temporaries
    return *this;
  }
};
```

Expression templates

If only we had a special class ...

- ... which stored references to `X`, `Y` and `Z`
- and had an **`operator`**`[]` which returns `a*X[i]+2*a*Y[i]+3*a*Z[i]`
- We could equip our `vec` class with a special assignment operator taking this special class as the right hand side

```
template <typename T>
class vec {
  template <class XPR>
  vec & operator=(const XPR & r)
  {
    for (size_t i=0;i<size();++i) {
      dat[i]=r[i]; // and r[i] returns a*X[i]+2*a*Y[i]+3*a*Z[i]
    } // One single loop, no temporaries
    return *this;
  }
};
```

- We need a different special class for every expression we have to evaluate

Expression templates

- If we make a class like :

```
template <typename LHS, typename RHS>
class vecsum {
    const LHS & lhs;
    const RHS & rhs;
public:
    vecsum(const LHS & l, const RHS & r) : lhs(l), rhs(r) {
        assert(l.size()==r.size());
    }
    auto operator[](size_t i) const { return lhs[i] + rhs[i]; }
    size_t size() const { return lhs.size(); }
};
```

- We can define the sum of two `vecxpr` objects to be a `vecsum` type

```
template <typename LHS, typename RHS>
vecsum<LHS,RHS> const operator+(const LHS & v1, const RHS & v2)
{
    return vecsum<LHS,RHS>(v1,v2);
}
```

Expression templates

- If we try `vec1+vec2`, no evaluation happens, and we get a `vecsum<vec,vec>` object
- But, if we try `vec1+54` or `34+"dino"`, we get nonsensical compound objects
- If we write our **`operator`**+ like :

```
 template <typename LHS, typename RHS>
vecsum<LHS,RHS> const operator+(const expr<LHS> & v1, const expr<RHS> & v2)
{
    return vecsum<LHS,RHS>(v1,v2);
}
```

, we can prevent the template from matching anything other than objects which match the pattern `expr<something>`

- If we further want composability of the operations, we need `vecsum<LHS,RHS>` to also match the pattern `vecxpr<something>`

Expression templates

Design with CRTP

- By creating a base template `vecxpr` to use as a base for all expressions of `vec` objects

```
template <class Derived> struct vecxpr {
  inline size_t size() const {
    return static_cast<Derived const &>(*this).size();
  }
  inline const auto operator[](size_t i) const {
    return static_cast<Derived const &>(*this)[i];
  }
  operator Derived & () {
    return static_cast<Derived&>(*this);
  }
  operator const Derived & () const {
    return static_cast<const Derived&>(*this);
  }
};
```

, we can prevent the template from matching anything other than objects which match the pattern `vecxpr<something>`

Expression templates

Design with CRTP

- We make our expression classes like `vecsum` inherit from the template `vecxpr` instantiated on themselves:

```
 template <typename T1, typename T2>
class vecsum : public vecxpr<vecsum<T1,T2>> {
  const T1 & lhs;
  const T2 & rhs;
public:
  using value_type=typename T1::value_type;
  vecsum(const vecxpr<T1> & l, const vecxpr<T2> & r) : lhs(l), rhs(r) {
    assert(l.size()==r.size());
  }
  const auto operator[](size_t i) const { return lhs[i] + rhs[i]; }
  size_t size() const { return lhs.size(); }
};
```

Expression templates

Design with CRTP

- We make our expression classes like `vecsum` inherit from the template `vecxpr` instantiated on themselves:

```
 template <typename T1, typename T2>
class vecsum : public vecxpr<vecsum<T1,T2>> {
  const T1 & lhs;
  const T2 & rhs;
public:
  using value_type=typename T1::value_type;
  vecsum(const vecxpr<T1> & l, const vecxpr<T2> & r) : lhs(l), rhs(r) {
    assert(l.size()==r.size());
  }
  const auto operator[](size_t i) const { return lhs[i] + rhs[i]; }
  size_t size() const { return lhs.size(); }
};
```

- **`operator`**+ can now be written as:

```
template <typename T1, typename T2>
vecsum<T1,T2> const operator+(const vecxpr<T1> & v1, const vecxpr<T2> & v2)
{
    return vecsum<T1,T2>(v1,v2);
}
```

Expression templates

Design with CRTP

- We also make the original `vec` class inherit from `vecxpr`

```
template <typename T> class vec : public vecxpr<vec<T>> {
  std::vector<T> dat;
public:
  using value_type = T;
  vec(size_t n) : dat(n) {}
  inline const T operator[](size_t i) const { return dat[i]; }
  inline T & operator[](size_t i) { return dat[i]; }
  inline size_t size() const { return dat.size(); }
  inline size_t n_ops() const { return 0; }
  template <typename X>
  vec & operator=(const vecxpr<X> & y) {
    dat.resize(y.size());
    for (size_t i=0;i<y.size();++i) dat[i]=y[i];
    return *this;
  }
};
```

Expression templates

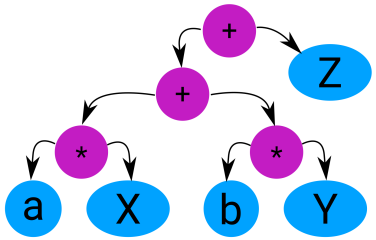
Design with CRTP

- We also make the original `vec` class inherit from `vecxpr`

```
template <typename T> class vec : public vecxpr<vec<T>> {
  std::vector<T> dat;
public:
  using value_type = T;
  vec(size_t n) : dat(n) {}
  inline const T operator[](size_t i) const { return dat[i]; }
  inline T & operator[](size_t i) { return dat[i]; }
  inline size_t size() const { return dat.size(); }
  inline size_t n_ops() const { return 0; }
  template <typename X>
  vec & operator=(const vecxpr<X> & y) {
    dat.resize(y.size());
    for (size_t i=0;i<y.size();++i) dat[i]=y[i];
    return *this;
  }
};
```

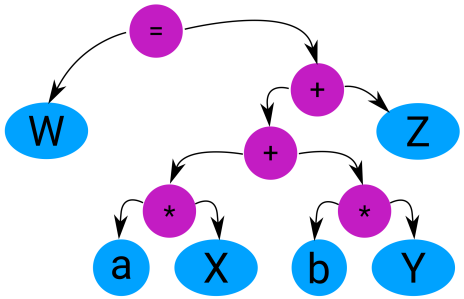
- Notice the special assignment operator from an expression!

Expression templates




```
a*X + b*Y + Z;
```

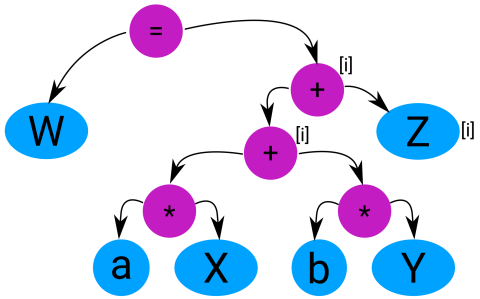
```
vecsum<
  vecsum<
    vecscl<vec<double>>,
    vecscl<vec<double>>
  >,
  vec<double>
> ({{a,X},{b,Y}},Z);
// Let's call this type EXPR
```




```
W = a*X + b*Y + Z;
```

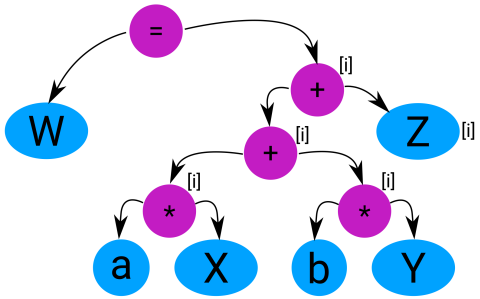
```
vec<double> &
vec<double>::operator=(const EXPR & E)
{
  dat.resize(E.size());
  for (size_t i=0;i<E.size();++i)
    dat[i]=E[i];
  return *this;
}
```

Expression templates




```
W = a*X + b*Y + Z;
```

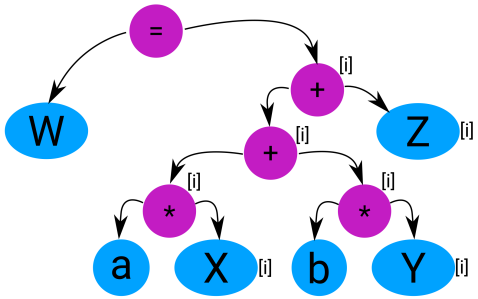
```
vec<double> &
vec<double>::operator=(const EXPR & E)
{
  dat.resize(E.size());
  for (size_t i=0;i<E.size();++i)
    dat[i]=E[i];
  return *this;
}
```




```
W = a*X + b*Y + Z;
```

```
const auto
vecsum<L,R>::operator[](size_t i) const {
  return lhs[i] + rhs[i];
}
```

Expression templates




```
W = a*X + b*Y + Z;
```

```
vec<double> &
vec<double>::operator=(const EXPR & E)
{
  dat.resize(E.size());
  for (size_t i=0;i<E.size();++i)
    dat[i]=E[i];
  return *this;
}
```

```
const auto
vecscl<T>::operator[](size_t i) const {
  return lhs * rhs[i];
}
```

Expression templates

- Elegant high level syntax

Expression templates

- Elegant high level syntax
- Reduce temporaries

Expression templates

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- Loop fusion

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- Delayed evaluation: apply algorithmic optimizations on the entire expression, e.g.,

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  - Evaluate `Matrix1 * Matrix2 * Vector` as `Matrix1 * (Matrix2 * Vector)`

Expression templates

- Elegant high level syntax
- Reduce temporaries
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- Delayed evaluation: apply algorithmic optimizations on the entire expression, e.g.,
  - Evaluate `Matrix1 * Matrix2 * Vector` as `Matrix1 * (Matrix2 * Vector)`
  - Detect and eliminate cancelling operations, e.g., `Matrix_xpr1.transpose().transpose()`

Expression templates

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  - Use optimized low level kernels with assembler, intrinsics, calls to vendor libraries etc to do the work

Expression templates

- Elegant high level syntax
- Reduce temporaries
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- Delayed evaluation: apply algorithmic optimizations on the entire expression, e.g.,
  - Evaluate `Matrix1 * Matrix2 * Vector` as `Matrix1 * (Matrix2 * Vector)`
  - Detect and eliminate cancelling operations, e.g., `Matrix_xpr1.transpose().transpose()`
  - Use optimized low level kernels with assembler, intrinsics, calls to vendor libraries etc to do the work
- However, can greatly increase compilation times

Example 16:

In `examples/xtmp0`, you will find a program which takes two numbers N and a as command line arguments, and creates 4 arrays W, X, Y, Z of size N (user defined array type `vec`). It fills X, Y and Z with random numbers and then calculates $W = a * X + 2 * a * Y + 3 * a * Z$, and times this operation by repeating the calculation 10 times. Two implementations of the user defined array type `vec` can be found: `naive_vec.hh` and `xtmp_vec.hh`. Compile and run the program by alternating between the two headers. Study the code in `xtmp_vec.hh`, which illustrates the ideas presented here about expression templates.

Exercise 3:

Introduce your own matrix class in the set up used in `examples/xtmp0`, so that matrix vector multiplications can be parts of vector expressions and `M1*M2*v` is evaluated as two matrix vector products rather than a matrix-matrix product followed by a matrix vector product.

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Linear Algebra

Linear algebra

- Operations on matrices, vectors, linear systems etc.
- Data parallel, simple numerical calculations
- Can be hand coded, but taking proper account of available CPU instructions, memory hierarchy etc is hard
- Libraries with standardized syntax for wide applicability
- Excellent vendor libraries are available on HPC systems

Eigen: A C++ template library for linear algebra

- Include only library. Download from http://eigen.tuxfamily.org/, unpack in a location of your choice, and use. Nothing to link.
- Small fixed size to large dense/sparse matrices
- Matrix operations, numerical solvers, tensors ...
- Expression templates: lazy evaluation, smart removal of temporaries

```
// examples/Eigen/eigen1.cc
#include <iostream>
#include <Eigen/Dense>
using namespace Eigen;
using namespace std;
int main()
{
  MatrixXd m=MatrixXd::Random(3,3);
  m = (m+MatrixXd::Constant(3,3,1.2))*50;
  cout << "m =" << endl << m << endl;
  VectorXd v(3);
  v << 1, 2, 3;
  cout <<"m * v ="<<endl<<m*v<<endl;
}
```

```
$ G -eigen eigen1.cc
```

- Explicit vectorization
- Elegant API

Eigen: matrix types

- `MatirxXd` : matrix of arbitrary dimensions
- `Matrix3d` : fixed size 3×3 matrix
- `Vector3d` : fixed size 3d vector
- Element access `m(i,j)`
- Output `std::cout << m << "\n";`
- Constant : `MatrixXd::Constant(a,b,c)`
- Random : `MatrixXd::Random(n,n)`
- Products : `m * v` or `m1 * m2`
- Expressions : `3 * m * m * v1 + u * v2 + m * m * m`
- Column major matrix :

```
Matrix<float, 3, 10, Eigen::ColMajor>
```

Eigen: matrix operations

```
#include <iostream>
#include <Eigen/Dense>
using namespace std;
using namespace Eigen;
int main()
{
   Matrix3f A;
   Vector3f b;
   A << 1,2,3,  4,5,6,  7,8,10;
   b << 3, 3, 4;
   cout << "Here is the matrix A:\n" << A << endl;
   cout << "Here is the vector b:\n" << b << endl;
   Vector3f x = A.colPivHouseholderQr().solve(b);
   cout << "The solution is:\n" << x << endl;
}
```

- Blocks `m.block(start_r, start_c, nr, nc)`, or `m.block<nr,nc>(start_r, start_c)`
-
```
   SelfAdjointEigenSolver<Matrix2f> eigensolver(A);
   if (eigensolver.info() != Success) abort();
   cout << "Eigenvalues << eigensolver.eigenvalues() << endl;
```

Eigen: examples

Example 17:

There are a few example programs using Eigen in the folder `examples/Eigen`. Read the programs `eigen0.cc` and `eigen1.cc`. To compile, use `G -eigen program.cc`.

Exercise 4:

The folder `examples/Eigen` contains a matrix multiplication example, `matmul.cc` using Eigen. Compare with a naive version of a matrix multiplication program, `matmul_naive.cc`, by compiling and running both programs. Try different matrix sizes. Then, you can use a parallel version of the Eigen matrix multiplication by recompiling with `-fopenmp`.

Exercise 5:

The file `exercises/PCA` has a data file with tabular data. Each column represents all measurements of a particular type, while each row is a different trial. In each row, the first column, x_{i0}, represents a pseudo-time variable. Write a program using Eigen to perform a Principal Component Analysis on this data set, ignoring the first column. Hint:
if $X_i = [x_{i1}, x_{i2}, ...x_{im}]$ is the data of row i, the covariance matrix is defined as,

$$C_{ab} = \frac{1}{(n-1)} \sum_k x_{ka} x_{kb}$$

The principal components of the data are obtained by right multiplying the data matrix by the matrix whose columns are the eigen vectors of the matrix C_{ab}, conventionally ordered by decreasing eigenvalues.

Eigen: some issues

```
Eigen::Tensor<double, 3> epsilon(3,3,3);
epsilon.setZero();
Eigen::SGroup<Eigen::AntiSymmetry<0,1>, Eigen::AntiSymmetry<1,2>> sym;
sym(epsilon, 0, 1, 2) = 1;
```

- "Standard C++98": Operates within the obsolete constraints of old C++

Eigen: some issues

```
Eigen::Tensor<double, 3> epsilon(3,3,3);
epsilon.setZero();
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- "Standard C++98": Operates within the obsolete constraints of old C++
- Evolution of the language standard opens up new possibilities. Case in point: `Eigen::Tensor` (example above) elegantly leverages variadic templates

Eigen: some issues

```
Eigen::Tensor<double, 3> epsilon(3,3,3);
epsilon.setZero();
Eigen::SGroup<Eigen::AntiSymmetry<0,1>, Eigen::AntiSymmetry<1,2>> sym;
sym(epsilon, 0, 1, 2) = 1;
```

- "Standard C++98": Operates within the obsolete constraints of old C++
- Evolution of the language standard opens up new possibilities. Case in point: `Eigen::Tensor` (example above) elegantly leverages variadic templates
- Performance lags behind vendor libraries (e.g., Intel MKL on JURECA) for strictly BLAS problems. But note: Eigen can use MKL behind the scenes.

Exercise 6:

Recompile the Eigen matrix multiplication example, this time to use intel MKL library (on JURECA). The procedure is described here : `http://eigen.tuxfamily.org/dox/TopicUsingIntelMKL.html`. On JURECA, using the Eigen module used in the course, you can do the following:
`G -eigen-mkl matmul.cc`. Run it on one node of JURECA and compare with the previous exercise.

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Threading Building Blocks

TBB: Threading Building Blocks I

- Parallel programming constructs for the end user
- Template library rather than language extensions
- Provides utilities like `parallel_for`, `parallel_reduce` to simplify the most commonly used structures in parallel programs
- Provides scalable concurrent containers such as vectors, hash tables and queues for use in multi-threaded environments
- No direct support for vector parallelism. But can be combined with auto-parallelisation and **`#pragma`** `simd` etc from Cilk
- Supports complex models such as pipelines, data flow and unstructured task graphs
- Scalable memory allocation, thread local storage

TBB: Threading Building Blocks II

- Low level synchronisation tools like mutexes and atomics
- Work stealing task scheduler
- http://www.threadingbuildingblocks.org
- Structured Parallel Programming, Michael McCool, Arch D. Robinson, James Reinders

Using TBB

- Include `tbb/tbb.h` in your file
- Public names are available under the namespaces `tbb` and `tbb::flow`
- You indicate "available parallelism", scheduler may run it in parallel if resources are available
- Unnecessary parallelism will be ignored

parallel invoke

```
void prep(Population &p);
void iomanage();
tbb::parallel_invoke(prep,iomanage,
     [other]{
       other.some_member();
});
```

Example 18: examples/TBB/-parallel_invoke.cc

Compile with `G -tbb parallel_invoke.cc`

- A few adhoc tasks which do not depend on each other
- Runs them in parallel
- waits until all of them are finished

TBB task groups

```
struct Equation {
  void solve();
};

std::list<Equation> equations;
tbb::task_group g;
for (auto eq : equations)
  g.run([]{eq.solve();});

g.wait();
```

- Run an arbitrary number of callable objects in parallel

TBB task groups

```
struct Equation {
  void solve();
};

std::list<Equation> equations;
tbb::task_group g;
for (auto eq : equations)
  g.run([]{eq.solve();});

g.wait();
```

- Run an arbitrary number of callable objects in parallel
- In case an exception is thrown, the task group is cancelled

TBB task scheduler

```
int main(int argc, char *argv[])
{
  size_t nthreads=std::stoul(argv[1]);
  //tbb::task_scheduler_init nit;
  tbb::task_scheduler_init nit(nthreads);
  haha();
}
void haha()
{
  ...
  tbb::parallel_invoke(a,b,c,d,e);
}
void a()
{
  tbb::parallel_for(...);
}
```

- Task scheduler: manages tasks, maps them to threads etc.
- Initializes the task scheduler
- Default constructor creates threads as needed while resources permit
- One scheduler is enough

Parallel for loops

- Template function modelled after the **`for`** loops, like many STL algorithms

```
tbb::parallel_for(first,last,f);
// parallel equivalent of
// for (auto i=first;i<last;++i) f(i);

tbb::parallel_for(first,last,stride,f);
// parallel equivalent of
// for (auto i=first;i<last;i+=stride)
//   f(i);

tbb::parallel_for(first,last,
                  [captures](anything){
  //Code that can run in parallel
});
```

Parallel for loops

- Template function modelled after the **`for`** loops, like many STL algorithms
- Takes a callable object as the third argument

```
tbb::parallel_for(first,last,f);
// parallel equivalent of
// for (auto i=first;i<last;++i) f(i);

tbb::parallel_for(first,last,stride,f);
// parallel equivalent of
// for (auto i=first;i<last;i+=stride)
//   f(i);

tbb::parallel_for(first,last,
                  [captures](anything){
  //Code that can run in parallel
});
```

Parallel for loops

- Template function modelled after the **`for`** loops, like many STL algorithms
- Takes a callable object as the third argument
- Using lambda functions, you can expose parallelism in sections of your code

```
tbb::parallel_for(first,last,f);
// parallel equivalent of
// for (auto i=first;i<last;++i) f(i);

tbb::parallel_for(first,last,stride,f);
// parallel equivalent of
// for (auto i=first;i<last;i+=stride)
//   f(i);

tbb::parallel_for(first,last,
                  [captures](anything){
  //Code that can run in parallel
});
```

Parallel for with ranges

- Splits `range` into smaller ranges, and applies `f` to them in parallel

```
tbb::parallel_for(0,1000000,f);
// One parallel invocation for each i!
tbb::parallel_for(range,f);

// A type R can be a range if the
// following are available
R::R(const R &);
R::~R();
bool R::is_divisible() const;
bool R::empty() const;
R::R(R & r,split);//Split constructor
```

Parallel for with ranges

- Splits `range` into smaller ranges, and applies `f` to them in parallel
- Possible to optimize `f` for sub-ranges rather than a single index

```
tbb::parallel_for(0,1000000,f);
// One parallel invocation for each i!
tbb::parallel_for(range,f);

// A type R can be a range if the
// following are available
R::R(const R &);
R::~R();
bool R::is_divisible() const;
bool R::empty() const;
R::R(R & r,split);//Split constructor
```

Parallel for with ranges

- Splits `range` into smaller ranges, and applies `f` to them in parallel
- Possible to optimize `f` for sub-ranges rather than a single index
- Any type satisfying a few design conditions can be used as a range

```
tbb::parallel_for(0,1000000,f);
// One parallel invocation for each i!
tbb::parallel_for(range,f);

// A type R can be a range if the
// following are available
R::R(const R &);
R::~R();
bool R::is_divisible() const;
bool R::empty() const;
R::R(R & r,split);//Split constructor
```

Parallel for with ranges

- Splits `range` into smaller ranges, and applies `f` to them in parallel
- Possible to optimize `f` for sub-ranges rather than a single index
- Any type satisfying a few design conditions can be used as a range
- Multidimensional ranges possible

```
tbb::parallel_for(0,1000000,f);
// One parallel invocation for each i!
tbb::parallel_for(range,f);

// A type R can be a range if the
// following are available
R::R(const R &);
R::~R();
bool R::is_divisible() const;
bool R::empty() const;
R::R(R & r,split);//Split constructor
```

Parallel for with ranges

```
tbb::blocked_range<int> r{0,30,20};
assert(r.is_divisible());
blocked_range<int> s{r};
//Splitting constructor
assert(!r.is_divisible());
assert(!s.is_divisible());
```

- `tbb::blocked_range<int>(0,4)` represents an integer range 0..4

Parallel for with ranges

```
tbb::blocked_range<int> r{0,30,20};
assert(r.is_divisible());
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//Splitting constructor
assert(!r.is_divisible());
assert(!s.is_divisible());
```

- `tbb::blocked_range<int>(0,4)` represents an integer range 0..4
- `tbb::blocked_range<int>(0,50,30)` represents two ranges, 0..25 and 26..50

Parallel for with ranges

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tbb::blocked_range<int> r{0,30,20};
assert(r.is_divisible());
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```

- `tbb::blocked_range<int>(0,4)` represents an integer range 0..4
- `tbb::blocked_range<int>(0,50,30)` represents two ranges, 0..25 and 26..50
  - So long as the size of the range is bigger than the "grain size" (third argument), the range is split

Parallel for with ranges

```
void dasxpcy_tbb(double a, std::vector<double> &x, std::vector<double> &y) {
  tbb::parallel_for(tbb::blocked_range<int>(0,x.size()),
                    [&](tbb::blocked_range<int> r){
    for (size_t i=r.begin();i!=r.end();++i) {
      y[i]=a*sin(x[i])+cos(y[i]);
    }
  });
}
```

- `parallel_for` with a range uses split constructor to split the range as far as possible, and then calls f(range), where `f` is the functional given to `parallel_for`

Parallel for with ranges

```
void dasxpcy_tbb(double a, std::vector<double> &x, std::vector<double> &y) {
  tbb::parallel_for(tbb::blocked_range<int>(0,x.size()),
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```

- `parallel_for` with a range uses split constructor to split the range as far as possible, and then calls f(range), where `f` is the functional given to `parallel_for`
- It is unlikely that you wrote your useful functions with ranges compatible with `parallel_for` as arguments

Parallel for with ranges

```
void dasxpcy_tbb(double a, std::vector<double> &x, std::vector<double> &y) {
  tbb::parallel_for(tbb::blocked_range<int>(0,x.size()),
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    }
  });
}
```

- `parallel_for` with a range uses split constructor to split the range as far as possible, and then calls f(range), where `f` is the functional given to `parallel_for`
- It is unlikely that you wrote your useful functions with ranges compatible with `parallel_for` as arguments
- But with lambda functions, it is easy to fit the parts!

Example 19: TBB parallel for demo

The program `examples/dasxpcy.cc` demonstrates the use of parallel for in TBB. It is a slightly modified version of the commonly used DAXPY demos. Instead of calculating $y = a * x + y$ for scalar a and large vectors x and y, we calculate $y = a * sin(x) + cos(y)$. To compile, you need to load your compiler and TBB modules, and use them like this:

```
G -I$TBB_INCLUDE_DIR dasxpcy.cc -L$TBB_LIBRARY_DIR -ltbb -ltbbmalloc
```

2D ranges

```
void f(size_t i, size_t j);
tbb::blocked_range2d<size_t> r{0,N,0,N};
tbb::parallel_for(r,[&](tbb::blocked_range2d<size_t> r){
  for (size_t i=r.rows().begin();i!=r.rows().end();++i) {
    for (size_t j=r.cols().begin();j!=r.cols().end();++j) {
      f(i,j);
    }
  }
});
```

- `rows()` is an object with a `begin()` and an `end()` returning just the integer row values in the range. Similarly: `cols()` ...

2D ranges

```
void f(size_t i, size_t j);
tbb::blocked_range2d<size_t> r{0,N,0,N};
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```

- `rows()` is an object with a `begin()` and an `end()` returning just the integer row values in the range. Similarly: `cols()` ...
- 2D range can also be split

2D ranges

```
void f(size_t i, size_t j);
tbb::blocked_range2d<size_t> r{0,N,0,N};
tbb::parallel_for(r,[&](tbb::blocked_range2d<size_t> r){
  for (size_t i=r.rows().begin();i!=r.rows().end();++i) {
    for (size_t j=r.cols().begin();j!=r.cols().end();++j) {
      f(i,j);
    }
  }
});
```

- `rows()` is an object with a `begin()` and an `end()` returning just the integer row values in the range. Similarly: `cols()` ...
- 2D range can also be split
- The callable object argument should assume that the original 2D range has been split many times, and we are operating on a smaller range, whose properties can be accessed with these functions.

Parallel reductions with ranges

```
T result = tbb::parallel_reduce(range, identity, subrange_reduction, combine);
```

- `range` : As with parallel for
- `identity` : Identity element of type T. The type determines the type used to accumulate the result
- `subrange_reduction` : Functor taking a "subrange" and an initial value, returning reduction
- `combine` : Functor taking two arguments of type T and returning reduction over them over the subrange. Must be associative, but not necessarily commutative.

Parallel reduce with ranges

```
double inner_prod_tbb(std::vector<double> & x, std::vector<double> & y) {
  return tbb::parallel_reduce(
      tbb::blocked_range<int>(0,n), // range
      double{}, // identity
      [&](tbb::blocked_range<int> &r,float in){
        return std::inner_product(x.begin()+r.begin(),x.begin()+r.end(),
                                  y.begin()+r.begin(),in);
      }, // subrange reduction
      std::plus<double>{} // combine
  );
}
```

- With TBB ranges, we can use blocked implementations with hopefully vectorisable calculations in subranges

Parallel reduce with ranges

```
double inner_prod_tbb(std::vector<double> & x, std::vector<double> & y) {
  return tbb::parallel_reduce(
      tbb::blocked_range<int>(0,n), // range
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      [&](tbb::blocked_range<int> &r,float in){
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                                  y.begin()+r.begin(),in);
      }, // subrange reduction
      std::plus<double>{} // combine
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}
```

- With TBB ranges, we can use blocked implementations with hopefully vectorisable calculations in subranges
- Two functors are required, either of which could be lambda functions

Parallel reduce with ranges

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double inner_prod_tbb(std::vector<double> & x, std::vector<double> & y) {
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      tbb::blocked_range<int>(0,n), // range
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                                  y.begin()+r.begin(),in);
      }, // subrange reduction
      std::plus<double>{} // combine
  );
}
```

- With TBB ranges, we can use blocked implementations with hopefully vectorisable calculations in subranges
- Two functors are required, either of which could be lambda functions
- Important to add the contribution of initial value in subrange reductions

Example 20: TBB parallel reduce

The program `tbbreduce.cc` is a demo program to calculate an integral using `tbb::parallel_reduce`. Check how lambda functions are used to do the integral. What kind of speed up do you see relative to the serial version ? Does it make sense considering the number of physical cores in your computer ?

Atomic variables

- "Instantaneous" updates

```
std::array<double,N> A;
tbb::atomic<int> index;

void append(double val)
{
  A[index++]=val;
}
```

Atomic variables

- "Instantaneous" updates
- Lock-free synchronization

```
std::array<double,N> A;
tbb::atomic<int> index;

void append(double val)
{
  A[index++]=val;
}
```

Atomic variables

- "Instantaneous" updates
- Lock-free synchronization
- For `tbb::atomic<T>`, T can be integral, enum or pointer type

```
std::array<double,N> A;
tbb::atomic<int> index;

void append(double val)
{
  A[index++]=val;
}
```

Atomic variables

- "Instantaneous" updates
- Lock-free synchronization
- For `tbb::atomic<T>`, T can be integral, enum or pointer type
- If `index==k` simultaneous calls to `index++` by n threads will increase `index` to `k+n`. Each thread will use a distinct value between `k` and `k+n`

```
std::array<double,N> A;
tbb::atomic<int> index;

void append(double val)
{
  A[index++]=val;
}
```

But it is important that we use the return value of `index++` in the threads!

Enumerable thread specific

```
tbb::enumerable_thread_specific<double> E;
double Eglob=0;
double f(size_t i, size_t j);
tbb::blocked_range2d<size_t> r{0,N,0,N};
tbb::parallel_for(r,[&](tbb::blocked_range2d<size_t> r){
  auto & eloc=E.local();
  for (size_t i=r.rows().begin();i!=r.rows().end();++i) {
    for (size_t j=r.cols().begin();j!=r.cols().end();++j) {
      if (j>i) eloc += f(i,j);
    }
  }
});
Eglob=0;
for (auto & v : E) {Eglob+=v;v=0;}
```

- Thread local "views" of a variable

Enumerable thread specific

```
tbb::enumerable_thread_specific<double> E;
double Eglob=0;
double f(size_t i, size_t j);
tbb::blocked_range2d<size_t> r{0,N,0,N};
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    }
  }
});
Eglob=0;
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```

- Thread local "views" of a variable
- behaves like an STL container of those views

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  auto & eloc=E.local();
  for (size_t i=r.rows().begin();i!=r.rows().end();++i) {
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- Thread local "views" of a variable
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- Member function `local()` gives a reference to the local view in the current thread

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  auto & eloc=E.local();
  for (size_t i=r.rows().begin();i!=r.rows().end();++i) {
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    }
  }
});
Eglob=0;
for (auto & v : E) {Eglob+=v;v=0;}
```

- Thread local "views" of a variable
- behaves like an STL container of those views
- Member function `local()` gives a reference to the local view in the current thread
- Any thread can access all views by treating it as an STL container

Example 21: Reduction with enumerable thread specific

You can use the `enumerable_thread_specific` and `parallel_for` to implement reduction. The program `examples/tbbreduce1.cc` demonstrates this.

TBB allocators

- Dynamic memory allocation in a multithreaded program must avoid conflicts from **`new`** calls from different threads
- Reduce global memory locks

TBB allocators

- Interface like `std::allocator`, so that it can be used with STL containers. E.g.,
  `std::vector<T, tbb::cache_aligned_allocator<T>>`
- `tbb::scalable_allocator<T>` : general purpose scalable allocator type, for rapid allocation from multiple threads
- `tbb::cache_aligned_allocator<T>` : Allocates with cache line alignment. As a consequence, objects allocated in different threads are guaranteed to be in different cache lines.

Concurrent containers

```
#include <tbb/concurrent_vector.h>

auto v=tbb::concurrent_vector<int>(N,0);

tbb::parallel_for(v.range(),[&](tbb::concurrent_vector::range_type r){
    //...
});
```

- Random access by index

Concurrent containers

```
#include <tbb/concurrent_vector.h>

auto v=tbb::concurrent_vector<int>(N,0);

tbb::parallel_for(v.range(),[&](tbb::concurrent_vector::range_type r){
    //...
});
```

- Random access by index
- Multiple threads can grow container and add elements concurrently

Concurrent containers

```
#include <tbb/concurrent_vector.h>

auto v=tbb::concurrent_vector<int>(N,0);

tbb::parallel_for(v.range(),[&](tbb::concurrent_vector::range_type r){
    //...
});
```

- Random access by index
- Multiple threads can grow container and add elements concurrently
- Growing the container does not invalidate any iterators or indexes

Concurrent containers

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#include <tbb/concurrent_vector.h>

auto v=tbb::concurrent_vector<int>(N,0);

tbb::parallel_for(v.range(),[&](tbb::concurrent_vector::range_type r){
    //...
});
```

- Random access by index
- Multiple threads can grow container and add elements concurrently
- Growing the container does not invalidate any iterators or indexes
- Has a `range()` member function for use with `parallel_for` etc.

Exercise 7: N particle systems with pairwise interactions

Use the `enumerable_thread_specific` and `parallel_for` to calculate the pairwise interactions in an N-particle system.

Thrust

NVIDIA Thrust

```
#include <thrust/host_vector.h>
#include <thrust/device_vector.h>
#include <thrust/generate.h>
#include <thrust/sort.h>
#include <thrust/copy.h>
#include <cstdlib>
using namespace thrust;
int main()
{
  // generate 32 M random numbers on
  // the host
  host_vector<int> h_vec(32 << 20);
  generate(h_vec.begin(), h_vec.end(),
           rand);

  // transfer data to the device
  device_vector<int> d_vec = h_vec;
  // sort data on the device (846M keys
  // per second on GeForce GTX 480)
  sort(d_vec.begin(), d_vec.end());
  // transfer data back to the host
  copy(d_vec.begin(), d_vec.end(),
       h_vec.begin());
}
```

- Template library like STL or TBB for CUDA, with great documentation.

NVIDIA Thrust

```
#include <thrust/host_vector.h>
#include <thrust/device_vector.h>
#include <thrust/generate.h>
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int main()
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  sort(d_vec.begin(), d_vec.end());
  // transfer data back to the host
  copy(d_vec.begin(), d_vec.end(),
       h_vec.begin());
}
```

- Template library like STL or TBB for CUDA, with great documentation.
- Provides an elegant high level syntax to clearly express the intent of the programmer

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  // per second on GeForce GTX 480)
  sort(d_vec.begin(), d_vec.end());
  // transfer data back to the host
  copy(d_vec.begin(), d_vec.end(),
       h_vec.begin());
}
```

- Template library like STL or TBB for CUDA, with great documentation.
- Provides an elegant high level syntax to clearly express the intent of the programmer
- The compiler translates the stated intents to efficient code for the GPU

NVIDIA Thrust

The bad

- Lag in supported C++ features => Syntax degradation to older practices.

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- NVIDIA GPUs only

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  - As of CUDA 8, C++14 is not supported in `.cu` files!
  - Only "experiental" support for even 6 year old C++11 version of lambda functions
- NVIDIA GPUs only

- Host exclusive C++14 code can be compiled directly with the underlying compiler, and combined inside a project with C++11 restricted `.cu` files containing `thrust` code

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  // transfer data back to the host
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}
```

- Example: `thrust::host_vector` and `thrust::device_vector` use the assignment operator to transfer data between the CPU and the GPU

NVIDIA Thrust

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- Thrust algorithms like `thrust::sort` have syntax like STL algorithms

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}
```

- Example: `thrust::host_vector` and `thrust::device_vector` use the assignment operator to transfer data between the CPU and the GPU
- Thrust algorithms like `thrust::sort` have syntax like STL algorithms
- Many data parallel general operations have their own algorithms: `transform`, `reduce`, `inclusive_scan`

Host and device vectors

```
#include <thrust/host_vector.h>
#include <thrust/device_vector.h>
#include <iostream>
int main()
{
  thrust::host_vector<int> H(4);
  for (int i=0;i<4;++i) H[i]=i;
  // resize H
  H.resize(2);
  std::cout << "H now has size "
      << H.size() << std::endl;
  // Copy host_vector H to
  // device_vector D
  thrust::device_vector<int> D = H;
  // elements of D can be modified
  D[0] = 99;
  D[1] = 88;
  // print contents of D
  for(int i = 0; i < D.size(); i++)
    std::cout << "D[" << i << "] = "
      << D[i] << std::endl;
}
```

- Containers `host_vector` and `device_vector` are designed similar to `std::vector`, but (as of CUDA 8.0), do not have initializer list constructors or new member functions of `std::vector` like `emplace_back`

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    std::cout << "D[" << i << "] = "
      << D[i] << std::endl;
}
```

- Containers `host_vector` and `device_vector` are designed similar to `std::vector`, but (as of CUDA 8.0), do not have initializer list constructors or new member functions of `std::vector` like `emplace_back`
- The overloaded assignment operators can copy data across devices

Other initialization options

```
// initialize all ten integers to 1
thrust::device_vector<int> D(10, 1);
// set the first seven elements to 9
thrust::fill(D.begin(), D.begin() + 7,
             9);
// initialize a host_vector with
// the first five elements of D
thrust::host_vector<int> H(D.begin(),
                           D.begin() + 5);
// set elements of H to 0, 1, 2, ...
thrust::sequence(H.begin(), H.end());
```

- Many algorithms to provide initial values, to serve different purposes.
- There is also `thrust::generate` which can call a functional for every element of the vector
- The type of the iterators tell the compiler which version of the respective algorithms to use. No run-time overhead

Example 22:

The example programs `examples/thrust/test0.cc` and `examples/thrust/test1.cc` contain the thrust code in the previous slides. Run them on JURECA using the following steps:

- Find out what CUDA modules are installed and load the most recent one you can find
- Compile using the `nvcc` compiler: `nvcc test0.cu`
- Try changing the file name to `test0.cc`
- Consult the information sheet distributed in the class room about how to run your programs on JURECA GPU nodes.

Thrust algorithms

```
device_vector<int> X(10),Y(10),Z(10);
// initialize X to 0,1,2,3, ....
sequence(X.begin(), X.end());
// compute Y = -X
thrust::transform(X.begin(), X.end(),
   Y.begin(), thrust::negate<int>());
// fill Z with twos
thrust::fill(Z.begin(), Z.end(), 2);
// compute Y = X mod 2
thrust::transform(X.begin(), X.end(),
             Z.begin(), Y.begin(),
             thrust::modulus<int>());
// replace all the ones in Y with 10
thrust::replace(Y.begin(),Y.end(),
                1,10);
// print Y
thrust::copy(Y.begin(), Y.end(),
std::ostream_iterator<int>(cout,"\n"));
```

- Host and device versions

Thrust algorithms

```
device_vector<int> X(10),Y(10),Z(10);
// initialize X to 0,1,2,3, ....
sequence(X.begin(), X.end());
// compute Y = -X
thrust::transform(X.begin(), X.end(),
   Y.begin(), thrust::negate<int>());
// fill Z with twos
thrust::fill(Z.begin(), Z.end(), 2);
// compute Y = X mod 2
thrust::transform(X.begin(), X.end(),
             Z.begin(), Y.begin(),
             thrust::modulus<int>());
// replace all the ones in Y with 10
thrust::replace(Y.begin(),Y.end(),
                1,10);
// print Y
thrust::copy(Y.begin(), Y.end(),
std::ostream_iterator<int>(cout,"\n"));
```

- Host and device versions
- A set of elementary functionals are available in `thrust/functional.h`

Thrust algorithms

```
device_vector<int> X(10),Y(10),Z(10);
// initialize X to 0,1,2,3, ....
sequence(X.begin(), X.end());
// compute Y = -X
thrust::transform(X.begin(), X.end(),
   Y.begin(), thrust::negate<int>());
// fill Z with twos
thrust::fill(Z.begin(), Z.end(), 2);
// compute Y = X mod 2
thrust::transform(X.begin(), X.end(),
             Z.begin(), Y.begin(),
             thrust::modulus<int>());
// replace all the ones in Y with 10
thrust::replace(Y.begin(),Y.end(),
                1,10);
// print Y
thrust::copy(Y.begin(), Y.end(),
std::ostream_iterator<int>(cout,"\n"));
```

- Host and device versions
- A set of elementary functionals are available in `thrust/functional.h`
- Notice the copy from a device vector to the ostream iterator!

Custom functionals for transforms

```
struct saxpy_functor {
  const float a;
  saxpy_functor(float _a) : a(_a) {}
  __host__ __device__
    float operator()(const float& x,
                     const float& y) const {
      return a * x + y;
    }
};
void saxpy_fast(float A,
      thrust::device_vector<float>& X,
      thrust::device_vector<float>& Y)
{
  // Y <- A * X + Y
  thrust::transform(X.begin(), X.end(),
                    Y.begin(), Y.begin(),
                    saxpy_functor(A));
}
```

- When pre-defined operations in `thrust/functional.h` do not suffice, we can write our own function objects
- The overloaded **`operator()`** must be marked with `__host__ __device__`

Custom functionals using placehoders

- For very simple operations, custom functionals can be generated inline using the `thrust::placehoders` namespace.

```
void saxpy_fast(float A,
      thrust::device_vector<float>& X,
      thrust::device_vector<float>& Y)
{
  // Y <- A * X + Y
  thrust::transform(X.begin(), X.end(),
                    Y.begin(), Y.begin(),
                    (A*_1 +_2));
}
```

- _1, _2 ... are placehoders
- Expressions involving placeholders yield a functional mapping its arguments sequencially to _1, _2 ...

Custom functionals using lambda functions

- In CUDA 8, you can also use C++11 (but not C++14) style lambda functions

```
void saxpy_fast(float A,
      thrust::device_vector<float>& X,
      thrust::device_vector<float>& Y)
{
  // Y <- A * X + Y
  thrust::transform(X.begin(), X.end(),
                    Y.begin(), Y.begin(),
                    [A] __host__ __device__
                    (double x, double y){
    return A * x + y;
  });
}
```

```
nvcc -std=c++11 --expt-extended-lambda\
  saxpy0.cu
```

- Can have many lines of code with loops etc like a normal function
- Reference capture (thankfully!) not allowed
- Note where we mark the lambda function to be for the host and device

Example 23: Placeholders and lambda functions

The example `examples/saxpy0.cu` shows how to use the placehoders with `thrust` algorithms for simple inline functionality. There is also a commented out version of the same thing done using a lambda function. The placeholder version is more compact, but the lambda version can have multiple statements, like a normal function.

Exercise 8: Mandelbrot set

The Mandelbrot set is the set of complex numbers c for which the function $f(z) = z^2 + c$ does not diverge when iterated from $z = 0$. An image representing the set can be created by generating the sequence $z_n = z_{n-1}^2 + c$ for each pixel in the image, by treating the x and y values of the pixel as the real and imaginary components of c. The sequence can be taken to have diverged if the magnitude of z exceeds 2. The program `exercises/mandelbrot.cc` does it, using the standard C++ library. Modify to do the computations using `thrust`.

Reductions

```
int sum=thrust::reduce(D.begin(),D.end(),
            (int)0,thrust::plus<int>());
int sum=thrust::reduce(D.begin(),D.end(),
            (int)0);
int sum=
    thrust::reduce(D.begin(),D.end());
int     result = thrust::count(vec.begin
      (),
              vec.end(), 1);
// thrust::count_if
// thrust::inner_product
float v=
   thrust::transform_reduce(d_x.begin(),
   d_x.end(),unary_op,init,binary_op) );
```

- Reductions require a binary operation and some initial value
- For convenience, variants like `count`, `count_if`, `inner_product` exist
- If a reduction is to follow a transform on the same data, `transform_reduce` offers an opportunity for "kernel fusion"

Partial sums, sorting, etc.

```
int data[6] = {1, 0, 2, 2, 1, 3};
inclusive_scan(data,data+6,data);
exclusive_scan(data,data+6,data);
// data is now {0, 1, 1, 3, 5, 6}
thrust::sort(A, A + N);
const int N = 6;
int    keys[N]={1,4,2,8,5,7};
char values[N]={'a','b','c','d',
                'e','f'};
thrust::sort_by_key(keys,keys+N,
                    values);
// keys is now   {1,2,4,5,7,8}
// values is now {'a','c','b',
                  'e','f','d'}
thrust::stable_sort(A,A+N,
          thrust::greater<int>());
```

- Frequently needed algorithms, which are not trivial to parallelize, have thrust implementations

Partial sums, sorting, etc.

```
int data[6] = {1, 0, 2, 2, 1, 3};
inclusive_scan(data,data+6,data);
exclusive_scan(data,data+6,data);
// data is now {0, 1, 1, 3, 5, 6}
thrust::sort(A, A + N);
const int N = 6;
int    keys[N]={1,4,2,8,5,7};
char values[N]={'a','b','c','d',
                'e','f'};
thrust::sort_by_key(keys,keys+N,
                    values);
// keys is now   {1,2,4,5,7,8}
// values is now {'a','c','b',
                  'e','f','d'}
thrust::stable_sort(A,A+N,
          thrust::greater<int>());
```

- Frequently needed algorithms, which are not trivial to parallelize, have thrust implementations
- Nicely hides low-level details and lets us work on the program logic

Partial sums, sorting, etc.

```
int data[6] = {1, 0, 2, 2, 1, 3};
inclusive_scan(data,data+6,data);
exclusive_scan(data,data+6,data);
// data is now {0, 1, 1, 3, 5, 6}
thrust::sort(A, A + N);
const int N = 6;
int    keys[N]={1,4,2,8,5,7};
char values[N]={'a','b','c','d',
                'e','f'};
thrust::sort_by_key(keys,keys+N,
                    values);
// keys is now   {1,2,4,5,7,8}
// values is now {'a','c','b',
                  'e','f','d'}
thrust::stable_sort(A,A+N,
          thrust::greater<int>());
```

- Frequently needed algorithms, which are not trivial to parallelize, have thrust implementations
- Nicely hides low-level details and lets us work on the program logic
- The high-level syntax is parsed at compile time, and reduced to efficient system specific implementations. Overhead exists, but it is low.

Thrust iterator library

```
thrust::constant_iterator<int> first(10);
first[0]   // returns 10
first[100] // returns 10
thrust::counting_iterator<int> first(10);
first[0]   // returns 10
first[1]   // returns 11
first[100] // returns 110
first = thrust::make_transform_iterator(vec.begin(), negate<int>());
...
last  = thrust::make_transform_iterator(vec.end(),   negate<int>());
thrust::reduce(first, last);   // returns -60 (i.e. -10 + -20 + -30)

thrust::device_vector<int> map(2);
map[0] = 3;
map[1] = 1;
thrust::device_vector<int> source(6);
source[0] = 10;
source[1] = 20;
...
int sum = thrust::reduce(thrust::make_permutation_iterator(source.begin(),
                         map.begin()),
                         thrust::make_permutation_iterator(source.begin(),
                         map.end()));
```

Thrust zip iterator and arbitrary transforms

```
  struct arbitrary_functor {
    template <typename Tuple>
    __host__ __device__ void operator()(Tuple t) {
        // D[i] = A[i] + B[i] * C[i];
        thrust::get<3>(t) = thrust::get<0>(t) +
               thrust::get<1>(t) * thrust::get<2>(t);
    }
};
int main() {
    // allocate storage
    thrust::device_vector<float> A(5), B(5), C(5), D(5);
    // initialize input vectors
    A[0] = 3;  B[0] = 6;  C[0] = 2;
    A[1] = 4;  B[1] = 7;  C[1] = 5;
    ...
    // apply the transformation
    thrust::for_each(thrust::make_zip_iterator(
               thrust::make_tuple(A.begin(), B.begin(), C.begin(), D.begin())),
                     thrust::make_zip_iterator(
               thrust::make_tuple(A.end(),B.end(),C.end(),D.end())),
                     arbitrary_functor());
    // print the output
    for(int i = 0; i < 5; i++)
        std::cout << A[i] << " + " << B[i] << " * "
                  << C[i] << " = " << D[i] << std::endl;
}
```

Thrust examples

Example 24:

Download the thrust library with examples using `git clone https://github.com/thrust/thrust.git`. In the example directory you have many interesting sample programs. In the remaining time in the course room, read and run a few samples. They are well documented, but you can ask for any necessary explanations.