Object-Oriented Programming for Scientific Computing

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Prerequisites and Objectives

Prerequisites

- Familiarity with at least one programming language
- At least procedural programming in C / C++
- Willingness to program in practice

Objectives

- Improved programming skills
- Introduction of modern programming techniques
- Strong focus on topics of relevance to Scientific Computing

Course Outline

General course outline:

Short recapitulation of basics	data types, functions, templates, classes, etc.
The C++ Standard Library	input/output, containers, iterators, algorithms, exceptions, etc.
Advanced topics	dynamic polymorphism, RAII, template meta programming, static polymorphism, SFINAE, etc.
C++11 features	smart pointers, lambda expressions, variadic templates, random numbers, chrono library, threads, etc.
C++14 features	generic lambdas, variable templates
C++17 features	guaranteed copy elision, structured bindings, fold expressions
Upcoming C++20 features	modules, concepts, ranges, coroutines

The baseline for the lecture is the C++11 standard, with changes due to C++14 and C++17 taken into account. The new features of the upcoming C++20 standard will be introduced where appropriate.

Lecture Website

Link: conan.iwr.uni-heidelberg.de/teaching/oopfsc_ws2020/

Content:

- Link to draft of official standard
- Literature recommendations and quick reference
- GitLab instructions (for exercises)
- Lecture slides (updated after each lecture)
- Exercise sheets (same as above)

MUESLI links (also listed on the lecture website):

- Registration: muesli.mathi.uni-heidelberg.de/user/register
- Course page: muesli.mathi.uni-heidelberg.de/lecture/view/1288

Exercises and Exam

Exercises:

- Will be completely online this semester (see homepage)
- Assistant: Stefan Meggendorfer ⟨stefan.meggendorfer@iwr.uni-heidelberg.de⟩
- New exercises every week: on the website after the lecture
- To be handed in right before the lecture on Wednesday
- Geared towards g++ and Linux
- Correction, grading etc. depends on course size

Exam:

- Probably in the last week of the semester (TBA)
- Mandatory for all participants
- 50% of the points in the exercises required for admission, plus active participation in discussion

Why C++?

A (non-exhaustive) list of programming languages for scientific computing:

Fortran (1957)	old (think punchcards) but still very relevant today (e.g., numerical linear algebra, legacy physics/astronomy codes)
C (1972)	widespread language for high-performance low-level programming (operating systems, compilers, ...)
C++ (1985)	started as "C with classes", newer iterations favor a style that is closer to, e.g., Python
Python (1990)	popular language with large ecosystem of numerical software libraries
Julia (2012)	relatively new language specifically designed for high-performance scientific computing

There are also several domain specific languages (DSL) that are strong in their respective domains, e.g.:
MATLAB (1984), R (1993)

Why C++?

Each language has its advantages and disadvantages, so which should be used for a course like this one?

Ideally, such a programming language for scientific computing ...

- is general-purpose, so no DSL
- produces highly efficient and portable programs
- provides a large ecosystem of numerical / scientific libraries
- has proven its suitability over the years
- has a large following, which provides support and makes it unlikely that the language will vanish
- can serve as a starting point to learn other, related languages

Why C++?

Fortran has a small community nowadays, is used for very specific applications, and its writing style has little overlap with the other aforementioned languages.

C is basically a subset of C++, apart from some technicalities.

Python would be a really good choice, but it is easier to move from C++ to Python than vice versa, and Python tends to hide some aspects of scientific programming that should be taught.

Julia is a relatively new language that is not yet in wide-spread use.

. . . which leaves us with C++ as a solid choice.

Versions of C++

The C++ language has evolved significantly over the last few years:

- "Classic" C++ code is officially known as C++98/03.
- Current versions of C++, i.e., C++11 with its relatively minor updates C++14 and C++17, have quite a different feel.
- In general, modern C++ constructs should be preferred wherever possible.
- But: these are often not covered in introductory courses.

We therefore start the lecture with a quick review of C++98/03, which is then used as starting point to discuss modern C++, how it evolved, and how it can be used to produce more readable and more maintainable code.

Evolution of C++

Classic C Style

```
// C-style fixed-length array
int fix[10] = {0,1,2,3,4,5,6,7,8,9};

// "fix" doesn't know its own size
for (int i = 0; i < 10; i++)
  if (fix[i] % 2 == 0)
    std::cout << fix[i] << " ";
std::cout << std::endl;

// C-style "variable-length" array
int* var = new int[n];
for (int i = 0; i < n; i++)
  var[i] = i;

// "var" isn't a real variable-length array:
// adding elems requires copying (or tricks)

// "var" doesn't know its own size
for (int i = 0; i < n; i++)
  if (var[i] % 2 == 0)
    std::cout << var[i] << " ";
std::cout << std::endl;

// oops, forgot to delete array: memory leak!
```

- C-style arrays are just references to contiguous blocks of memory (basically pointers to first entry)
- They don't follow value semantics: copies refer to same memory blocks
- Their length is not stored and has to be specified explicitly, inviting subtle errors
- Runtime fixed-length arrays aren't true variable-length arrays
- May lead to nasty memory leaks if they aren't explicitly deallocated

Evolution of C++

C++98/03

```
// C++ variable-length array
// from header <vector>
std::vector<int> var(n);
for (int i = 0; i < n; i++)
  var[i] = i;

// std::vector is a real variable-length array
var.push_back(n+1);

// no need to remember size of "var"
for (int i = 0; i < var.size(); i++)
  if (var[i] % 2 == 0)
    std::cout << var[i] << " ";
std::cout << std::endl;

// very general (also works for maps, sets,
// lists, ...), but reeeally ugly
for (std::vector<int>::const_iterator it
    = var.begin(); it != var.end(); ++it)
  if (*it % 2 == 0)
    std::cout << *it << " ";
std::cout << std::endl;
```

- C++ introduced `std::vector`, a true variable-length array, i.e., elements can be added and removed
- Vectors have value semantics: copies are deep copies
- A vector always knows its current size, no need to keep track
- Same performance as C-style arrays (drop-in replacement)
- Can be used in generic code via iterators (but leads to very verbose code)

Evolution of C++

C++11 / C++20

```cpp
// C++ variable-length array
std::vector<int> var(n);
// C++11: fill using algo from <numeric> header
std::iota(var.begin(),var.end(),0);

// C++11: range-based for loop
// hides ugly iterators
for (const auto& e : var)
  if (e % 2 == 0)
    std::cout << e << " ";
std::cout << std::endl;

// C++11: lambda expression (ad-hoc function)
auto even = [](int i){return i % 2 == 0;};

// C++20: filters and transforms
for (const auto& e : var
    | std::views::filter(even))
    std::cout << e << " ";
std::cout << std::endl;
```

- C++11 introduced range-based `for` loops, making iterator-based code much more readable
- C++20 will introduce filters and transforms that can operate on such loops, here in the example based on a C++11 lambda expression (ad-hoc function definition)

Evolution of C++

C++11

```cpp
// C-style fixed-length array
int fix[10] = {0,1,2,3,4,5,6,7,8,9};

// C++11: range-based for works with
// C-style arrays, but only for those
// with compile-time fixed length!
for (const auto& e : fix)
  if (e % 2 == 0)
    std::cout << e << " ";
std::cout << std::endl;

// C++11: modern array type from header <array>
std::array<int,10> fix2 = {0,1,2,3,4,5,6,7,8,9};

// no need to remember size of "fix2"
for (int i = 0; i < fix2.size(); i++)
  if (fix2[i] % 2 == 0)
    std::cout << fix2[i] << " ";
std::cout << std::endl;
```

- C++11 range-based `for` loops can be used with legacy arrays, since the compiler knows their size implicitly
- However, this doesn't work when the length is runtime-dependent!
- C++11 also introduced `std::array` as a drop-in replacement for fixed-length C-style arrays, with known size and value semantics like `std::vector`

Versions of C++

Which version of C++ should I learn / use?

- C++98/03 remains relevant due to (a) vast collections of legacy codebases resp. (b) programmers that still use old constructs and are set in their ways.
- C++11 is the current baseline and should be supported on virtually all platforms and compute clusters by now.
- C++14 is a minor update of C++11 and is also a safe choice. Most software projects should accept C++14 code by now.
- C++17 is a second minor update of C++11. This is perfectly fine for your own code, but keep in mind that large projects may be restricted to C++14 to support some architectures, see for example DUNE [1].
- C++20 is the upcoming new version and will bring major changes. This will become relevant in the near future.

[1] https://www.dune-project.org

Fundamental Concepts

The modern components of C++ are often built upon older constructs of the language, may serve as superior replacements for some of them, or both.

These fundamental concepts are:

- variables and types
- pointers and references
- control structures
- functions and templates
- classes and inheritance
- namespaces and structure

They are taught in practically any introductory course that is based on C++. We will quickly review them to make sure that everyone has the prerequisites for the following lectures.

Variables, Temporaries, Literals

C++, like any other programming language, concerns itself with the computation and manipulation of data.

This data represents many different things, from simple numbers and strings, to images and multimedia files, to abstract numerical simulations and their solutions.

Put simply, C++ knows three different categories of data:

Variables are names for locations where data is stored, e.g., `int i = 5;` referring to an integer value in memory.

Temporaries represent values that aren't necessarily stored in memory, e.g., intermediate values in compound expressions and function return values.

Literals are values that are explicitly mentioned in the source code, e.g., the number `5` above, or the string `"foo"`.

Data Types

C++ is a strongly-typed language, which means that each such representation of data, i.e., variable, temporary or literal, must have an associated data type.

This data type specifies how the underlying binary sequence encodes the data (semantics), and more importantly ensures that it isn't possible to accidentally misinterpret data or use it in the wrong context (type safety).

C++ has a number of built-in data types and allows the introduction of user-defined types based on certain rules. Each type is associated with a range of valid values of that type.

Fundamental Types

C++ provides a set of fundamental, or built-in, types, mostly inherited from C.

`void`:

A type that has no valid values. Represents "nothing" (e.g., as return type), sometimes "anything" (when using pointers).

`nullptr_t`:

A type with one value, `nullptr`, indicating an invalid pointer. Introduced to make pointer handling safer.

Fundamental Types

`bool` :

Two values, `true` and `false`, for standard Boolean algebra (truth values).

`char` et al.:

ASCII characters, also similar types for unicode support (`wchar_t`, `char16_t`, `char32_t`).

`int` et al.:

Integer numbers, with different ranges (`short`, `int`, `long`, `long long`) and signedness (`signed` and `unsigned`). `signed` is default and may be omitted. Also a standard type for container sizes (`std::size_t`), one for pointer differences (`std::ptrdiff_t`), and a very long list of fixed width types, like `std::int8_t`, etc.

Fundamental Types

`float` et al.:

Floating point numbers, with single precision (`float` : 32 bit), double precision (`double` : 64 bit), or extended precision (`long double` : usually 80 bit).

Nowadays, `double` is used as default floating point type if there is not a good reason to use something else.

Each of the integer and floating point types gives certain guarantees about the representable range. These and other properties can be queried using `std::numeric_limits` .

Introducing New Types

These built-in types can be combined with four different mechanisms to produce new type definitions. We already saw the first one, C-style arrays, the others are:

`enum` :

A user-defined set of constants:

```
enum Color = {red, blue, green};
```

These are actually integers behind the scenes, and may accidentally be used as such: prefer → scoped enums.

`struct` :

The cartesian product of some types, i.e., the set of all possible tuples of values:

```
struct PairOfInts {int a; int b;};
```

Introducing New Types

`union` :

The union set of some types, i.e., a type that can hold values from all specified types:

```
union IntOrChar {int c; char d;};
```

Unions don't store the type they currently contain, which is dangerous: consider → variants instead.

The resulting data types may then be used in further type definitions, e.g., structs as members of other structs, or data types that are augmented with additional components using → inheritance.

Examples from DUNE

Whenever possible, we will have a quick look at real-world code from the DUNE project[2], preferably from the PDELab subproject[3].

```
// classic enum defining boundary types for a domain
enum Type { Dirichlet=1, Neumann=-1, Outflow=-2, None=-3 };

// modern C++11 enum for DG finite element basis definition
enum class QkDGBasisPolynomial
    {lagrange, legendre, lobatto, l2orthonormal};

// In C++, structs are actually just classes with
// public attributes, we therefore refer to class
// examples in that regard.

// DUNE currently contains no unions (which is a good thing!)
```

[2] https://www.dune-project.org
[3] https://www.dune-project.org/modules/dune-pdelab

Pointers

Each type `T`, whether built-in or user-defined, has an associated type `T*` (pointer to `T`) defined, with the meaning "address of a value of type `T` in memory".

```
int i = 5;
int* p = &i;

int* p2 = new int;
*p2 = 4;
delete p2;
```

- An ampersand `&` in front of a variable produces its address
- An asterisk `*` in front of a pointer *dereferences* the pointer, providing access to the variable itself
- The keyword `new` can be used to acquire a slot in memory that is unnamed, i.e., not associated with a variable

It is imperative to release such memory with `delete` after it is no longer needed. Doing so too early leads to nasty bugs, forgetting to do so causes memory leaks. A possible solution are → smart pointers.

References

In constrast to C, C++ introduces a second indirection that serves a similar purpose: references `T&`. While pointers simply refer to some memory, and may be modified to point to other locations, references are always an alias for an existing entity.

```
int a = 5;
int& b = a; // b is an alias for a
b = 4;      // this changes a as well
```

Note that the symbol `&` is used in two different contexts, first to take addresses of variables and second to specify reference types. This is a bit unfortunate, but can no longer be changed (both constructs have seen widespread use over the last few decades).

Rvalue References

The third kind of indirection in C++ is the rvalue reference `T&&`, introduced in C++11. Ordinary references `T&` are now also known as lvalue references to distinguish the two concepts.

The (oversimplified) definitions of lvalue and rvalue are:

- lvalue: could be on the lefthand side of an assignment, is an actual entity, occupies memory and has an address
- rvalue: could be on the righthand side of an assignment, temporary and ephemereal, e.g., intermediate values or literals

Such rvalue references are mostly restricted to two use cases: as forwarding references in → range-based `for` loops, and as a vital component of the implementation of → move semantics.

Const-Correctness

The type of variables, pointers and references may be marked as `const`, i.e., something that can't be modified. This guards against accidental modification (bugs), and makes programmers' intent clearer. Therefore, `const` should be used wherever possible.

```
int i = 5;          // may change later on
const int j = 4;    // guaranteed to stay 4
const int& k = i; // k can't be modified
i += 2;             // ... but this still changes k indirectly!

const int* p1 = &i;         // pointer to const int
int const* p2 = &i;         // same thing
int* const p3 = &i;         // constant pointer to modifiable int
int const* const p4 = &i; // const pointer to const int
```

Read right-to-left: `const` modifies what's left of it (think `int const i`), but the leftmost const may be put on the lefthand side for readability (`const int i`).

Selection (Conditionals)

Branches are a fundamental form of program flow control. An `if` statement consists of a condition, some code that is executed if that condition is fulfilled, and optionally other code that is executed if it isn't fulfilled:

```
if (i % 2 == 0)
  std::cout << "i is even!" << std::endl;
else
  std::cout << "i is odd!" << std::endl;
```

There is also a `switch` statement, but `if` is used significantly more often.

```
switch(color) // the Color enum we introduced earlier
{
  case red:   std::cout << "red"   << std::endl; break;
  case blue:  std::cout << "blue"  << std::endl; break;
  case green: std::cout << "green" << std::endl;
}
```

Repetition (Loops)

C++ provides two different kinds of loops, `for` and `while` loops. The former is executed a fixed number of times[4], while the latter is repeated until some condition is met.

```
for (int i = 0; i < 10; i++)
  std::cout << i << std::endl;

int j = 9;
while (j > 1)
{
  std::cout << j << std::endl;
  j /= 2; // half, rounded down
}
```

If `j` were one, the loop would be skipped completely. There is also a variant `do{...} while(...)` that runs at least once.

[4] in practice — on a technical level, `for` and `while` are perfectly equivalent

Jump Statements

Sometimes code becomes more readable if certain parts of a loop can be skipped. The `continue` statement can be used to skip the rest of the current loop iteration, while `break` exits the loop prematurely:

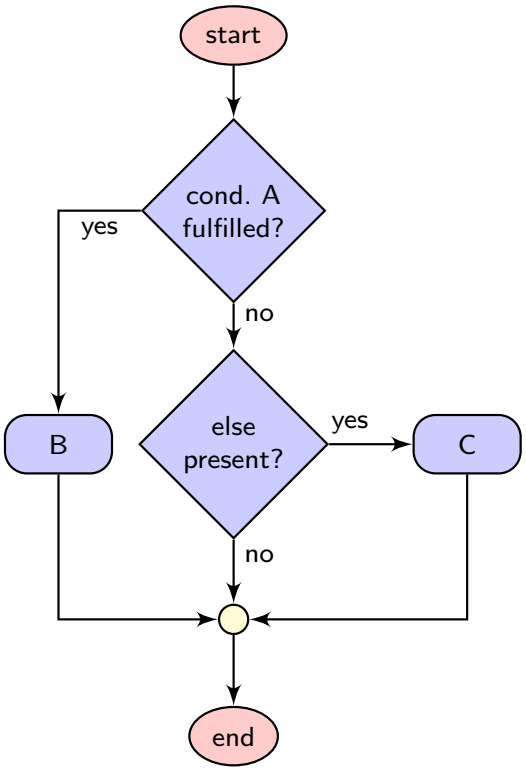
```
for (int i = 0; i < 100; i++)
{
  if (i % 2 == 0)
    continue;
  if (i > 10)
    break;
  // prints 1, 3, 5, 7, 9
  std::cout << i << std::endl;
}
```

These two statements jump to the end of the current iteration resp. the loop, i.e., they are constrained. C++ also has an unconstrained `goto` jump statement, but its use is strongly discouraged. There is one accepted use case: exiting several nested loops simultaneously (`break` would leave the innermost loop only).

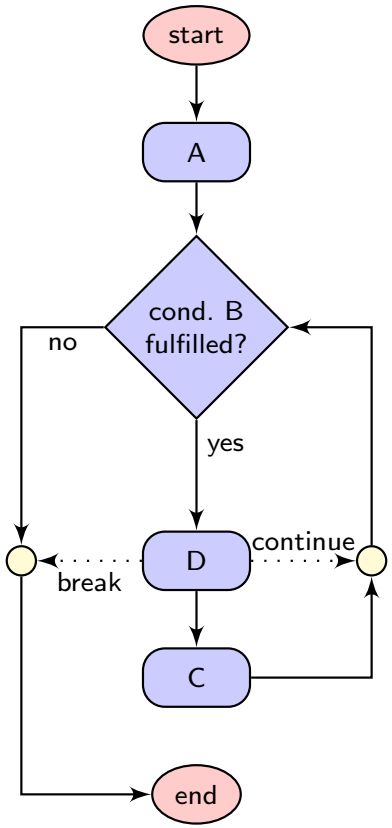
Diagram: Loops and Branches

The two fundamental control structures:

```
if (A) B; [[else C;]]
```




```
for (A;B;C) D;
```



The code

```
while (A) B;
```

is equivalent to

```
for (;A;) B;
```

and

```
do A while (B);
```

is equivalent to

```
A; while (B) A;
```

Subprograms (Functions)

A function is a subprogram that may be reused in different parts of the program, which reduces verbosity and helps in structuring the code. Functions have a name, zero or more arguments with fixed type, and a return type:

```
// expects one double argument, returns double
double square(double x)
{
  return x * x;
}

// expects an int and a double as args, returns nothing
void printSquares(int a, double b)
{
  std::cout << square(a) << " and " << square(b) << std::endl;
}
```

The special type `void` indicates a function that doesn't return anything. Such functions typically have side effects (I/O, or modifications to their arguments).

Call-by-Reference

C++ is one of the languages that always create copies of arguments when a function is called (call-by-value). This means that local changes to these variables don't modify the originals. In some other languages, the local names refer to the actual memory locations that were passed to the function (call-by-reference).

To emulate this behavior in C++, one passes a pointer or reference instead[5]:

```
// modifies its argument
void square(int* i)
{
  *i = *i * *i;
}

// prefer references: code is more readable
void square(int& i)
{
  i = i * i;
}
```

[5] There's still a copy (of the pointer/reference), but it refers to the original location.

Call-by-Reference

Call-by-reference is also often used when a function should return more than one value: one emulates this by modifying one or more reference arguments. C++17 and later standards provide → guaranteed copy elision and → structured bindings as a better alternative.

For large entities (e.g., vectors, matrices) it often makes sense to pass them by reference even if they should not be modified, since this avoids costly copy operations (both in terms of runtime and memory use):

```
// directly access original vector,
// but guarantee that it isn't modified
int sum(const std::vector<int>& vec)
{
  int out = 0;
  for (int i = 0; i < vec.size(); i++)
    out += vec[i];

  return out;
}
```

Default Arguments

C++ supports default arguments for functions. Arguments with defaults may then be omitted when calling the function[6]. This simplifies the function interface when these arguments have certain values most of the time:

```
void print(const std::vector<int>& vec, std::string sep = ", ",
           std::string pre = "(", std::string post = ")")
{
  std::cout << pre;
  for (int i = 0; i < vec.size() - 1; i++)
    std::cout << vec[i] << sep;
  if (!vec.empty())
    std::cout << vec.back();
  std::cout << post;
}
```

A call `print(v)` will then use a default layout, but other variants can be used if desired.

[6] That's why they always come last: to keep the call unambigious.

Function Overloading

C++ offers function overloading, i.e., using the same name for several different functions, as long as each function call is uniquely determined by the arguments (including handling of default arguments).

```
int maximum(int a, int b)
{
  if (a > b)
    return a;
  return b;
}

// a default argument for c would have to be
// smaller than any possible integer
int maximum(int a, int b, int c)
{
  return maximum(maximum(a,b),c);
}
```

Operator Overloading

C++ provides a large assortment of operators, i.e., tokens that are placed inline to specify some operation, like assignment (`a = b`), arithmetics (`a + b`), or comparison (`a < b`).

Most of these operators can also be defined for custom data types like `struct PairOfInts {int a; int b;};` . The definition works like that of an ordinary function overload:

```
PairOfInts operator+(const PairOfInts& p1, const PairOfInts& p2)
{
  return PairOfInts{p1.a + p2.a, p1.b + p2.b};
}
```

Given this definition, the following two expressions produce the same result:

```
// function call syntax
Pair p3 = operator+(p1,p2);
// operator syntax
Pair p4 = p1 + p2;
```

Function Pointers

In addition to the usual pointers, C++ also knows pointers to functions, e.g., `int (*f)(int)`, a pointer called `f` for functions expecting and returning `int`. To simplify notation, the asterisk `*` and ampersand `&` may be omitted when referring to function pointers and addresses of functions.

Using function pointers, functions may be used as arguments of other functions:

```
int square(int i)
{
  return i * i;
}

int applyTwice(int f(int), int i) // optional "*" omitted
{
  return f(f(i)); // no "*" allowed in call syntax
}

// computes pow(7,4), optional "&" omitted when taking address
std::cout << applyTwice(square,7) << std::endl;
```

Example from DUNE

I have found only one instance of function pointers in DUNE (*but it's hard to search for...*).

This code creates custom MPI parallel operation handles for given data types and binary functions (specified as `Type` and `BinaryFunction` template parameters). The address of `operation` is used to pass the function the handle should represent.

A C-style cast is used to remove argument data types.

```
static MPI_Op get ()
{
  if (!op)
  {
    op = std::shared_ptr<MPI_Op>(new MPI_Op);
    MPI_Op_create((void (*)(void*, void*, int*,
        MPI_Datatype*))&operation,true,op.get());
  }
  return *op;
}

static void operation (Type *in, Type *inout,
    int *len, MPI_Datatype*)
{
  BinaryFunction func;

  for (int i=0; i< *len; ++i, ++in, ++inout) {
    Type temp;
    temp = func(*in, *inout);
    *inout = temp;
  }
}
```

The Main Function

The execution of a C++ program starts in the first line of a special function called `main`, and ends when its last line is reached. Every C++ program has to define exactly one such function.

The signature of the main function has to be one of

- `int main()` (this means command line arguments are ignored)
- `int main(int argc, char** argv)`
- `int main(int argc, char* argv[])`

The second and third variant have the same meaning: `argc` is the number of arguments, and `argv` an array of C-style strings.

The return value of `main` is an error code — not returning anything is equivalent to writing `return 0;` (implying success).

Templates

Often, one has to define the same functionality for several different data types. This can become tedious, both during initial implementation and when fixing bugs.

C++ provides a language feature for this, where all the different versions are auto-generated from a special construct, called a function template:

```
template<typename T>
  T square(T x)
  {
    return x * x;
  }
```

A function `square<T>` is then available for any type `T` that has a multiplication operator `*`:

```
int i    = square<int>(5);       // int version
float f  = square<float>(27.f)   // float version
double d = square<double>(3.14) // double version
```

Templates

Function definitions aren't the only use case for templates, one can also automate the generation of data types. These are known as class templates, since structs are a special case of classes in C++.

```
template<typename T>
  struct Pair {T a; T b;};

Pair<int> ip;   // a pair of ints
Pair<float> fp; // a pair of floats

// Pair<int> is a data type, and can be used as such
Pair<Pair<int>> ipp; // pair of pair of ints
```

Function templates and class templates were the only types of templates until C++14, when → variable templates were introduced.

Non-Type Template Parameters

Typically, one uses template parameters to introduce abstract types `T`, but there are also non-type template parameters. These can be used as compile-time constants:

```
// simple fixed-length vector
template<typename T, int n>
  struct Vector
  {
    enum {dim = n}; // knows its size
    T vals[n];
  }
```

An advanced use case for such non-type template parameters is → template meta programming, where function values and number sequences can be precomputed at compile time.

Template Template Parameters

In addition to types and values, one may also use templates themselves as arguments for other templates, so-called template template parameters. These can, e.g., be used to allow choosing between different implementations:

```
// accepts any template that expects a type and an int
template<template<typename,int> class V>
  double norm(const V<double,3>& vec);
```

One such level of templates-in-templates can be a very powerful tool, but you shouldn't overdo it:

```
template<template<typename> class U, typename T>
  struct Wrap {U<T> u;};

// just don't...
template<template<template<typename> class,typename> class W>
  struct Meta {W<Pair,double> w;};
```

Default Template Parameters

All three types of template parameters, i.e., types, non-type template parameters, and template template parameters, can have defaults, just like function arguments:

```
// use our vector struct by default
template<template<typename,int> class V = Vector>
  double norm(const V<double,3>& vec);

// generalization of our Pair struct
template<typename U, typename V = U>
  struct Pair {U a; V b;};

// provides special case for square matrices
template<int n, int m = n>
  struct Matrix
  {
    // "misuse" enum for defs at compile time
    enum {dim1 = n};
    enum {dim2 = m};

    // ...
  };
```

Parameters with defaults may be omitted, i.e., one can write `Pair<int>` (just as before!), or `Matrix<5>` for square matrices.

Renaming Types

C and C++ provide the keyword `typedef`, which may be used to introduce new names for types. It is actually a slight misnomer, since there is no real new definition[7]: they are akin to C++ references, but on the conceptual level of data types.

```
typedef unsigned long long int ull;
ull a = 12345678901234567890u; // huge unsigned int
```

While such new names can be introduced for any type, it is especially helpful for the types from template instantiations:

```
typedef Pair<Vector<double,3>,Vector<double,2>> VecPair3D2D;
```

In C++11 and above, consider using → type aliases instead, as they are more general and more readable.

[7] Note that `typedef struct{int a; int b;} PairOfInts;` *is* a valid definition, albeit a rather convoluted one.

Example from DUNE

A template with template template parameter and default parameters introducing

- an inner template `MatrixHelper`
- two typedefs: `size_type` and `type`
- an → alias template named `Pattern`

```
template<template<typename> class Container = Simple::default_vector,
         typename IndexType = std::size_t>
  struct SparseMatrixBackend
  {
    typedef IndexType size_type;

    //! The type of the pattern object passed to the GridOperator for pattern construction.
    template<typename Matrix, typename GFSV, typename GFSU>
    using Pattern = Simple::SparseMatrixPattern;

    template<typename VV, typename VU, typename E>
    struct MatrixHelper
    {
      typedef Simple::SparseMatrixContainer<typename VV::GridFunctionSpace,
              typename VU::GridFunctionSpace,Container, E, size_type> type;
    };
  };
```

Function Template Parameter Deduction

The specification of template parameters is often redundant when using function templates, because type template parameters are readily deduced from the function arguments. If this is the case, they can be omitted, and the call looks like a normal (non-template) function call:

```
template<typename T>
  T square(T x)
  {
    return x * x;
  }

int i    = square(5);   // short for square<int>
double d = square(27.); // short for square<double>
```

Note that sometimes this isn't possible:

```
// can't deduce return type from call
template<typename T>
  T generate();
```

Classes / Methods

The original name of C++ was "C with classes", so classes, objects and object-oriented programming are clearly an important part of C++.

While a classic C struct is simply an aggregation of data, C++ structs and classes typically contain methods, functions that are closely linked to the data and part of the type definition:

```
struct Vector2D
{
  std::array<double,2> comp;

  // const: method may be called for const vectors
  double norm() const
  {
    return std::sqrt(comp[0]*comp[0] + comp[1]*comp[1]);
  }
}

Vector2D v{{3,4}};
std::cout << v.norm() << std::endl; // prints 5
```

Access Specifiers

C++ provides three access specifiers:

`private` : accessible by the object itself *and other objects of the same class*

`protected` : like `private`, but additionally accessible in → derived classes.

`public` : always accessible

Sometimes it is helpful to exempt certain classes or functions from these restrictions using a `friend` declaration. This should be used sparingly, since it breaks encapsulation and exposes implementation details.

```
struct BankAccount
{
  // full access -- maybe not the best of ideas?
  friend class Customer;

  private:
    double balance; // hide this!
};
```

Encapsulation

The only difference between C++ structs and classes is default visibility: in a struct, everything is `public` by default (but may be declared `private`), and vice versa for classes.

The hiding of implementation details using `private` is known as encapsulation and is generally a good idea, mainly for the following reasons:

- ensures consistent state: in a plain struct, data is either `const` or open to arbitrary, potentially nonsensical, changes
- facilitates modularity: `private` components are unknown outside of the class itself, and may therefore be exchanged and modified at will
- improves communication of intent: anything marked `public` is part of the intended interface

Constructors

Data that was declared `private` is inaccessible outside of the class, so we need special `public` methods to initialize such data. These methods are called constructors. In C++, they have the same name as the class they belong to and are the only functions without return type.

```
class Vector2D
{
  std::array<double,2> comp;

  public:

  Vector2D() : comp{0,0} {};

  Vector2D(double a, double b)
    : comp{a,b}
  {};

  // ...
};
```

This (incomplete) class provides two constructors, one for arbitrary points, and one for the origin.

Why not use default arguments instead? Because then one could omit `b` while supplying `a` (design decision).

Constructors

There are three types of constructors with special names:

- The default constructor `T()` without arguments: called, e.g., when mass producing `vector` entries during initialization
- The copy constructor `T(const T&)`: has the task of creating a copy of the object specified in the function call
- The move constructor `T(T&&)`: like the copy constructor, but may cannibalize the original object (which should be left in some valid default state)

Converting Constructors

Any constructor that is not marked as `explicit` is a so-called converting constructor, and is called for implicit type conversions[8]. Assume we have defined

```
Matrix(double); // diagonal matrix, or constant matrix?
operator*(double, const Matrix&);          // scaling
operator*(const Matrix&, const Matrix&); // matrix multiplication
```

but not `operator*(const Matrix&, double)`. Then a call `a * 2.`, with `a` a `Matrix`, will call `Matrix(2.)` followed by matrix multiplication. This may lead to unexpected results.

If such conversions aren't intended, the constructor has to be marked:

```
explicit Matrix(double); // no implicit type conversions
```

[8] type promotions, like from `int` to `double` when needed

Conversion Operators

Closely linked to constructors are conversion operators. While converting constructors are used to convert to the class type, these operators are used to convert *from* the class type to some other specified type, mainly when

- the target type is a fundamental type
- the target type is some class provided by an external library

In both cases it is impossible to simply provide the right constructor for the target type.

Here, conversion operators can be employed instead:

```
struct Vector
{
  operator Matrix(); // implicit promotion to column matrix
  explicit operator double(); // only explicit conversion
  ...
}
```

Delegating Constructors

Function overloading can be used to forward function calls to other versions of the same function, e.g., to swap function arguments, or as in the `maximum` function we introduced, or as a form of mutual recursion.

Similarly, one may define delegating constructors which call other constructors:

```
// constructor for square matrices uses general constructor
Matrix(int n)
  : Matrix(n,n) // no further entries allowed
{}
```

Rules:

- The delegating constructor may not initialize anything itself (only call this second constructor)
- The calls cannot be recursive (at some point, initialization has to take place)
- The function body is executed after the other constructor has finished (thereby allowing local modifications)

Destructors

Destructors are the counterpart to constructors: they clean up data when an object goes out of scope and its lifetime ends. Most of the time explicitly declaring a destructor isn't necessary, but it is vitally important if, e.g., memory was allocated by the object:

```
class IntStorage
{
  int n;
  int* data;

  public:

  IntStorage(int n_)
    : n(n_), data(new int[n])
  {};

  // copies are neither forbidden
  // nor handled correctly
  // --> segmentation fault waiting to happen

  ~IntStorage()
  {
    delete data;
  }
};
```

The name of the constructor is the class name with a tilde `~` as prefix.

The correct use of destructors leads directly to the technique of → Resource Acquisition is Initialization (RAII).

Default Methods

For any type `T`, the compiler automatically generates several methods for us if applicable:

- default constructor `T()`
- default destructor `~T()`
- copy constructor `T(const T&)`
- copy assignment `T& operator=(const T&)`
- move constructor `T(T&&)`
- move assignment `T& operator=(T&&)`

In each case, the method is not created automatically if that is impossible, e.g., if the class is storing some reference, or if there are user-defined versions.

Default Methods

In the case of the default constructor `T()`, the presence of any user-defined constructors prevents its creation.

The move constructor and move assignment operator aren't created if any of the other mentioned methods except the default constructor has been user-defined.

The assignment `= default` as in

```
T() = default
```

can be used to explicitly state that not providing some method is actually intended and not a mistake, or force the generation of the default constructor in the presence of other constructors.

Rules of Zero and Five

The rule of zero states that it is often a good idea to implement *at most* some custom constructors and none of the aforementioned methods. This is concise and perfectly appropriate when the class is just a collection of data with some methods.

However, sometimes it is necessary to provide replacements for these methods, e.g., because the default copy methods perform flat copies of pointer structures.

The rule of five[9] states that if a user-defined copy constructor, copy assignment operator, move constructor, move assignment operator, or destructor is present, then it is very likely that all five should be explicitly defined: if one of these methods has to be specialized, then the underlying reason is typically relevant for all of them.

[9] formerly known as "rule of three", before move semantics were introduced

Deleted Methods

Returning to the `IntStorage` object, we have two different options:

- provide user-defined copy/move constructors and assignment operators to enable deep copy semantics
- simply prohibit the creation of copies of such objects

Let's go with the second option for the sake of argument. Before C++11, one would have implemented the methods to prevent their automatic generation, and then declared them `private`. Any attempt to copy such an object would then trigger a compilation error, but the construct is a rather poor choice in terms of communicating intent.

Since C++11, one can declare methods as deleted, preventing their automatic creation:

```
T(const T&) = delete;
T& operator=(const T&) = delete;
```

Mutable Members

In C++, declaring an object `const` doesn't mean that its representation (byte sequence) has to be immutable, just that any such changes are invisible from the outside. The keyword `mutable` marks members as modifiable in `const` methods:

```
class Matrix
{
    mutable bool detValid = false;
    mutable double det;

  public:

    double determinant() const
    {
      if (!detValid)
      {
        det = calcDet(); // expensive (private) helper function
        detValid = true;
      }
      return det;
    }
}
```

Note that any method that modifies the matrix has to set `detValid = false`!

Static Members

The keyword `static` indicates that something belongs to the abstract definition, not the concrete instance:

- In functions definitions, `static` variables belong to the function itself, not the current function call (and therefore persist across function calls)
- In class definitions, `static` variables and methods belong to the class itself, not the created objects (i.e., they are shared between all objects of this class)

In functions, `static` variables can serve as function "memory", e.g., in function generators. In classes, `static` members can be used to, e.g., count the number of instantiated objects, manage a common pool of resources (memory, threads, ...), or provide small private helper functions.

The Singleton Pattern

A design pattern using `static` is the singleton pattern, which creates a class that provides exactly one instance of itself and prevents the creation of further such objects.

This pattern tends to be overused. It should be restricted to situations where

- the notion of two such objects doesn't make sense under any circumstance
- the single instance needs to be accessible from everywhere in the program

Standard applications concern the centralized management of system resources:

- a centralized logging facility, printing queues, or network stacks
- thread and memory pools, or the graphical user interface (GUI)

The Singleton Pattern

Realization of the singleton pattern in C++:

```
class Singleton
{
  public:
    Singleton& getInstance()
    {
      // kept alive across function calls
      static Singleton instance;
      return instance;
    }

    // prevent creation of copies
    Singleton(const Singleton&) = delete;
    void operator=(const Singleton&) = delete;

  private:
    // only callable within getInstance()
    Singleton(){...}; // hide constructor
};

// in user code:
Singleton& singleton = Singleton::getInstance();
```

Example from DUNE

An application of the singleton pattern in DUNE:

```
class MPIHelper
{
  public:
  ...

    DUNE_EXPORT static MPIHelper&
        instance(int& argc, char**& argv)
    {
      // create singleton instance
      static MPIHelper singleton (argc, argv);
      return singleton;
    }

  ...
  private:
  ...

    MPIHelper(int& argc, char**& argv)
    : initializedHere_(false)
    {...}
    MPIHelper(const MPIHelper&);
    MPIHelper& operator=(const MPIHelper);
};
```

- Conceptually, there can be only one instance of the Message Passing Interface (MPI).
- Its initialization and finalization functions must be called *exactly once*, the singleton pattern guarantees this.
- Copy constructor and assignment operator have been hidden instead of deleted (pre-C++11 style).

Inheritance

Quite often, there is a natural relationship between several classes based on their purpose:

- Several matrix classes (dense vs. sparse, small vs. millions of entries, local vs. parallely distributed, hierarchically blocked or not,...)
- Different algorithms for maxtrix inversion / decomposition
- A range of solvers for nonlinear problems, spatial discretizations, time stepping schemes...

This relationship can be expressed using inheritance:

- Extend and augment existing classes
- Collect and maintain common code in base classes
- Express and enforce interfaces through $\rightarrow$ abstract base classes (ABCs)

Inheritance

Inheritance establishes a relationship between classes, one derived class and an arbitrary number of base classes (typically just one).

```
struct A1 {int a};
struct A2 {int a};

struct B : A1, A2 // B inherits from A1 and A2
{
  int b;

  B(int c1, int c2, int c3) : b(c1), A1::a(c2), A2::a(c3)
};
```

The class `B` is an extension of both `A1` and `A2`, and contains three ints (two `a`s, and one `b`), since it inherits all data members and methods from `A` and `B`.

Inside of `B` the two different `a`s have to be accessed via `A1::a` and `A2::a`, because the simple name `a` would be ambiguous.

Class Hierarchies

Derived classes may themselves have derived classes, leading to a hierarchy of data types:

```
struct A {int i};
struct B : A {int j}; // B IS-A A
struct C : B {int k}; // C IS-A B (and therefore an A)
```

Again, `i` can be accessed in `C`, possibly under the name `B::A::i` if `i` alone would be ambiguous.

Conceptually, this hierarchy always forms a tree:

```
struct D : B, C {int l}; // contains two independent A and B each
```

`B::j` and `C::B::j` are two independent variables! We will see more about this when discussing the → Deadly Diamond of Death and → virtual inheritance.

Access Specifiers in Inheritance

Access specifiers can also be used when specifying inheritance relationships, as in

```
class A : public B {...};
```

If this access specifier is omitted, it defaults to `public` for structs and `private` for classes[10].

Access rights combinations for inherited methods and data members:

...is inherited...	`public`ly	`protected`ly	`private`ly
`public`	`public`	`protected`	`private`
`protected`	`protected`	`protected`	`private`
`private`	—	—	—

[10] This is the reason why "`: public`" is typically used instead.

Public Inheritance

Public inheritance models the subtype relationship from entity-relationship models: a derived class object IS-A base class object, in the sense that it fulfills the same interface.

Possible examples of this are:

- A Circle IS-A Shape
- A DiagonalMatrix IS-A Matrix
- A NewtonSolver IS-A NonlinearSolver

An object of the derived class is expected to be a perfect replacement for objects of the base class. This puts additional responsabilities on the person implementing the derived class, e.g., code operating on pointers and references of the base class should continue to work for those pointing to objects of the derived class.

The Liskov Substitution Principle

In principle, the subtype (derived class) should exhibit the same behavior as the supertype (base class). However, this is hard to verify in general. The Liskov Substitution Principle (LSP) defines some constraints that are meant to aid in this task.

Methods that share a name with one of the methods of the base class (and thereby override them) should not lead to surprising behavior:

Contravariance of arguments The method may also accept supertypes of the original arguments[11].

Covariance of return types The method may return a subtype of the original return type[12].

Exception safety The method may only throw the original → exceptions or subtypes thereof.

[11] not available in C++

[12] in C++ only in the context of → dynamic polymorphism

The Liskov Substitution Principle

Additionally, the following things should hold:

Preconditions The subtype may not strengthen preconditions (put additional constraints on the environment where its methods are called).

Postconditions The subtype may not weaken postconditions (leave conditions unfulfilled that are always fulfilled by the supertype).

Invariants The subtype must honor invariants of the supertype (things that are generally true for its objects)

History constraint The subtype may not allow state changes that are impossible from the viewpoint of the supertype.

In short, the base class part of the derived class should perform according to expectations. `private` members becoming inaccessible in the derived class helps in this regard.

Is a Square a Rectangle?

According to the LSP, it depends on the concrete implementation whether a Square is indeed a Rectangle:

- If squares and rectangles are immutable (unchangable after their creation), or only provide a methods for scale adjustments and rotation/translation, then a Square can be a Rectangle.
- If changing the length of a Square would also change its width, then assumptions about the supertype Rectangle would be violated.
- Keeping the width constant instead means it fails at being a Square.
- Therefore, Squares cannot be Rectangles if the length and width of rectangles can be controlled independently.

Again: Is a DiagonalMatrix a Matrix?

Protected/Private Inheritance

Private inheritance implements one class in terms of another:

- the members of the base class become private members of the derived class
- this is invisible from outside of the class
- the derived class may access the public interface of the base class

Mostly equivalent to just storing the base class as a private member instead, except for so-called empty base class optimization.

Protected inheritance works the same, but the inheritance is visible to children of the derived class as well. Seldom used and few applications.

Examples from DUNE

DUNE currently contains

- of course a large number of instances of public inheritance,
- exactly one instance of protected inheritance,
- and a small handful of cases with private inheritance.

```
class MacroGrid
  : protected DuneGridFormatParser
{...}

template <int block_size, class Allocator=std::allocator<bool> >
class BitSetVector : private std::vector<bool, Allocator>
{...}

template<int k>
struct numeric_limits<Dune::bigunsignedint<k> >
  : private Dune::Impl::numeric_limits_helper
      <Dune::bigunsignedint<k> > // for access to internal state of bigunsignedint
{...}
```

- `MacroGrid` and descendants may access internal `DuneGridFormatParser`
- `BitsetVector` is implemented using `std::vector`, but one may not be used as replacement for the other

Code Structure

We have now reviewed the fundamental building blocks of C++, and finish this section with a short look at code structure. C++ supports a range of tools that can be used to structure code bases and make large collections of code more maintainable:

- header files and the accompanying header guards to structure the concrete file layout and maintain code dependencies
- source files to provide implementations separate from declarations, thereby guaranteeing stable interfaces while allowing modification of implementation details
- namespaces to structure code on the conceptual level and prevent name clashes between different libraries

C++20 will introduce → modules as known from other programming languages, which will significantly improve importing other C++ libraries and exporting one's own constructs as a library.

Header Files

By convention, C++ code is separated into two different types of files:

- header files (`.hh`), containing declarations and interfaces
- source files (`.cc`), containing definitions and implementations

Both types of files are needed to build a given code project, but only the header files are necessary when writting code that should link against some external library.

Templates typically go against this convention, with their complete definition put into header files: the definition is needed during template instantiation, and without it dependent code could only use a given, fixed set of predefined and preinstantiated variants.

Header Guards

The `#include` preprocessor statement simply includes raw text from header files, recursively if necessary:

- Typically, header files are included several times within a program (e.g., `<iostream>`, `<vector>`, etc.).
- This would lead to redefinitions, and therefore compilation errors.
- Even without such errors, reparsing of these files would lead to long parse times, especially when considering header files including other header files.

Therefore, use header guards:

```
#ifndef HEADER_HH // only read file if not yet defined...
#define HEADER_HH // ...and define to prevent second read

... // actual header content (only parsed once)

#endif // HEADER_HH // reminder what is closed here
```

Namespaces

The one definition rule (ODR) of C++ demands that names are unambiguous:

- local definitions take precedence over those from enclosing scopes
- providing two differing definitions for the same name with the same visibility is forbidden

This leads to problems when

- a certain name should be reused in different parts of a very large program
- by coincidence, two (or more) external libraries define the same name

Solution: encapsulate libraries, sublibraries, and independent project parts using namespaces.

Namespaces

A simple namespace example:

```
namespace Outer
{
  namespace Inner
  {
    struct Data{};
  }
}
```

In this example, the `struct Data` is known as

- `Data`, `Inner::Data`, or `Outer::Inner::Data` in the innermost scope
- `Inner::Data` or `Outer::Inner::Data` in the outer scope
- only `Outer::Inner::Data` in the rest of the program

Example from DUNE

In DUNE, a namespace called (fittingly) `Dune` encapsulates the whole project. This namespace is used for the core modules.

Downstream modules like PDELab typically introduce subnamespaces, e.g., `Dune::PDELab`, for their own classes and functions. This way, these modules may use names that would otherwise collide with each other or parts of the core modules.

```
#ifndef DUNE_PDELAB_NEWTON_NEWTON_HH
#define DUNE_PDELAB_NEWTON_NEWTON_HH
...
namespace Dune
{
  namespace PDELab
  {
    // Status information of Newton's method
    template<class RFType>
    struct NewtonResult : LinearSolverResult<RFType>
    {
      ...
    }
    ...
  } // end namespace PDELab
} // end namespace Dune
#endif // DUNE_PDELAB_NEWTON_NEWTON_HH
```

The Standard Library

The Standard Library is a set of classes and functions that is part of the C++ language standard. It provides most of the common "tools of the trade": data structures and associated algorithms, I/O and file access, exception handling, etc. The components are easily recognized because they are in the `std` namespace.

Large parts of the Standard Library were already available in C++98/03 and are based on the Standard Template Library (STL), which is the library where common container classes like `std::vector` originate from. For this reason, it is still sometimes called "the STL".

Other parts were introduced in C++11 and later standards, often originating in the Boost C++ Libraries, a well-known set of open-source libraries that provide advanced utility classes and templates.

The Standard Library

We are going to discuss the following older parts of the Standard Library in detail:

- input and output streams
- containers (a.k.a. data structures) and iterators
- algorithms and functors
- companion classes (pair and tuple)
- exceptions

C++11 additions like → smart pointers, → random number generation, → threads, and → regular expressions will be discussed inat a later point, and the same holds for the → filesystems library from C++17.

Note that one usually has to include a certain header for a library feature to be available, e.g., `#include <iostream>` for I/O, or `#include <vector>` for `std::vector`.

Input / Output

C++ provides stream-based I/O: each stream is an abstraction for some source and/or destination of data, and each such stream is used in the same way, whether it represents standard C I/O, the content of a file, or simply the content of some string.

The relevant types are:

`[i,o,io]stream`	generic input, output, or bidirectional I/O stream
`[i,o,io]fstream`	specialization for reading / writing files
`[i,o,io]sstream`	sprecialization for strings as data sources/sinks

Input / Output

There are four predefined global variables for standard C I/O:

`cin`	standard C input stream
`cout`	standard C output stream
`cerr`	standard C error stream, unbuffered
`clog`	standard C error stream, buffered

For larger programs it is good practice not to write to these streams directly, since extraneous output can make it difficult to use the software in new contexts and other projects. Instead, one writes into intermediate stream objects, which may then redirect the data at their discretion.

Input / Output

The standard way of using streams are the well-known `<<` and `>>` operators, maybe with some I/O modifiers like floating-point formatting. Additionally, there are also special types of → iterators available that make a more or less seamless interaction with container classes possible.

If it should be possible to read and/or write an object from/to a stream (serialization[13]), one has to specialize the stream operators.

- Use free functions, because the stream is the left-hand side operand
- `friend` declaration, because we need access to the object internals

```
struct Streamable
{
  // ...

  // return streams to facilitate operator chaining
  friend std::istream& operator>>(std::istream& is, const Streamable& s);
  friend std::ostream& operator<<(std::ostream& os, const Streamable& s);
};
```

[13] https://isocpp.org/wiki/faq/serialization

Example from DUNE

```
//! Print a std::array
template<typename Stream, typename T,
    std::size_t N>
inline Stream& operator<<(Stream& stream,
    const std::array<T,N>& a)
{
  stream<<"[";
  if(N>0)
  {
    for(std::size_t i=0; i<N-1; ++i)
      stream<<a[i]<<",";
    stream<<a[N-1];
  }
  stream<<"]";
  return stream;
}
```

This code defines an output format for `std::array` as long as the stored type `T` itself can be printed.

The stream is returned to the caller, which enables operator chaining as in

```
std::cout << a1
          << " "
          << a2
          << std::endl;
```

Sequential Containers

C++ provides three different types of containers (data structures): sequences, container adaptors, and associative containers. They are the C++ versions of common and well-known data structures (array, linked list, tree, hash map, etc.).

The elements of container objects all have the same type, specified as a template parameter. This restriction can be somewhat lifted through → dynamic polymorphism. Since C++17 one may also use a → variant, or the → `std::any` class as element type.

The simplest type of container is a sequence, where the elements are associated with an integer index (either explicitly or implicitly).

Sequential Containers

C++ provides the following sequences:

array	array with fixed size and random access
vector	array with variable size and random access
deque	double-ended queue with random access
list	doubly linked list
forward_list	singly linked list

```
std::vector<int> a(3,5); // array [5,5,5]
std::vector<int> b{3,5}; // array [3,5]
std::list<double> c;     // empty doubly-linked list
```

Container Adaptors

In C++, a container adaptor implements some data structure in terms of another. Three such adaptors are provided:

stack	LIFO (last in, first out) structure
queue	FIFO (first in, first out) structure
priority_queue	a priority queue (surprise!)

```
std::stack<double> a;           // stack based on deque
std::stack<int,std::vector> b; // stack based on vector
std::queue<int,std::list> c;   // queue based on list
```

Associative Containers

In contrast to sequential containers, which are indexed by integers, associative containers may have an arbitrary index type. This index is associated with a value, and the container can be searched for this key, producing the value if the key is found.

C++ knows four sorted associative containers:

set	key is unique and identical to its associated value
multiset	like set, but key may appear multiple times
map	key is unique, value is pair of index and some mapped type
multimap	like map, but key may appear multiple times

The keys of these sorted containers need to be equipped with a strict weak ordering relation. The containers are typically implemented using red-black trees.

Associative Containers

Additionally, C++ also provides unsorted associative containers. While the sorted ones typically use trees internally, the unsorted ones are usually based on hash tables.

Each sorted container has an unsorted counterpart:
unordered_set, unordered_multiset, unordered_map, and unordered_multimap.

These unsorted containers are more universally applicable, since they don't need the underlying ordering relation. However, the elements appear in random order (based on the hash function in practice).

Unsorted containers tend to be faster than sorted containers but may be worse if there are many collisions in the hash function. For certain applications the guaranteed worst-case performance of sorted containers may be an important feature.

Complexity Guarantees

An important part of the container library are the accompanying complexity guarantees. Any implementation of C++ has to provide methods with certain upper bounds on performance. For the most part, these follow naturally from the default underlying data structures.

- Accessing an element of a `vector` is in $\mathcal{O}(1)$, and adding an element at the end is amortized[14] $\mathcal{O}(1)$, worst-case $\mathcal{O}(N)$, where N is the number of elements.
- Accessing an element of a `list` is in $\mathcal{O}(N)$, and adding or deleting elements is $\mathcal{O}(1)$ anywhere in the list.
- Operations on sorted associative containers are typically in $\mathcal{O}(\log N)$.
- For unsorted associative containers this is replaced with amortized $\mathcal{O}(1)$, worst-case $\mathcal{O}(N)$.

A table with all the container methods is available online[15], and complexity guarantees are linked from there.

[14] averaged over many method calls

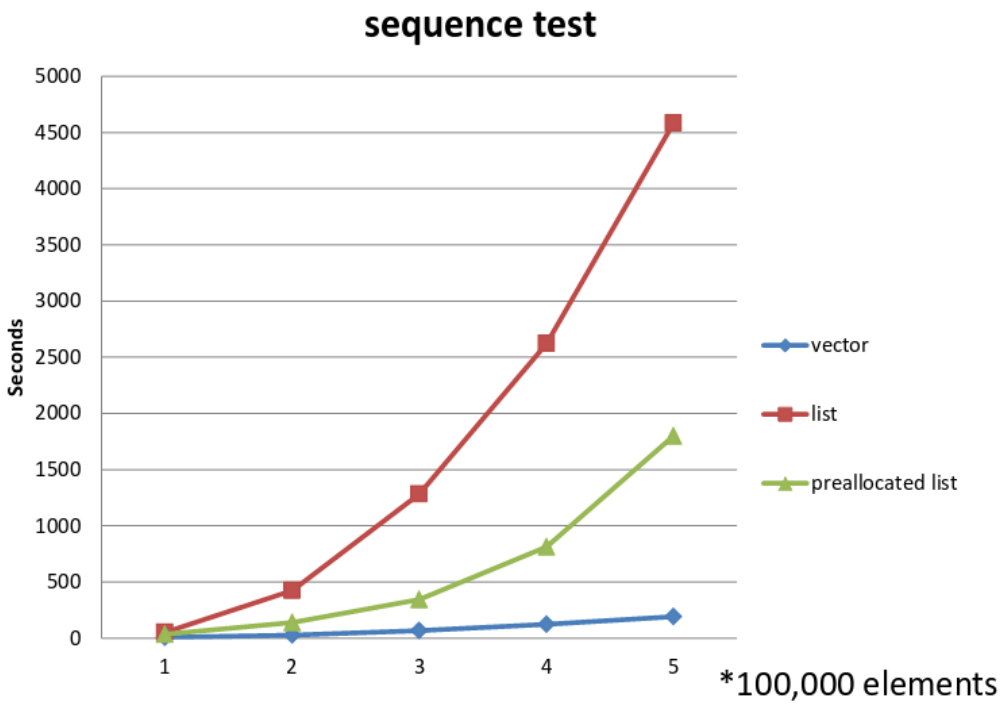
[15] https://en.cppreference.com/w/cpp/container

Sequence Test: Vector vs. List

Task by J. Bentley and B. Stroustrup (Element Shuffle):

- For a fixed number N, generate N random integers and insert them into a sorted sequence.
  Example:
  - 5
  - 1, 5
  - 1, 4, 5
  - 1, 2, 4, 5
- Remove elements at random while keeping the sequence sorted.
  Example:
  - 1, 2, 4, 5
  - 1, 4, 5
  - 1, 4
  - 4
- For which N should a `list` be used, and in which cases a `vector`?

Sequence Test: Vector vs. List



Source: B. Stroustrup

Potentially suprising results:

- Despite random insertion / deletion, `vector` is faster by an order of magnitude
- Linear search for both containers, despite bisection being available for `vector` (!)
- Search completely dominates move required by `vector`
- Non-optimized `list` performs one allocation / deallocation per element (!)

Use vector as default — and if not, back up assumptions with measurements

Iterators

The main way to interact with containers is via iterators, which are generalizations of the pointer concept, i.e., objects that can be dereferenced (`*`) and advanced (`++`). For each container type `T`, there is:

- an associated type `T::iterator`, for read / write access to the container
- an associated type `T::const_iterator`, providing read-only access
- a method `begin()`, which returns an iterator pointing to the first element
- a method `end()`, returning an iterator one position past (!) the last element
- equivalent methods `cbegin()` and `cend()` for read-only access

The element order is defined by the index for sequences, the keys for sorted containers, and the hash function for unsorted containers. There are also additional types / methods that reverse this order (`rbegin()`, `rend()`, etc.).

Iterators

Using iterators, one can write functions that work for different containers:

```
template<typename T>
  void print(const T& cont)
  {
    for (typename T::const_iterator it
        = var.begin(); it != var.end(); ++it)
      std::cout << *it << " ";
    std::cout << std::endl;
  }
```

- The keyword `typename` is used inside templates to specify that a dependent name (identifier that depends on at least one template parameter) refers to a type, since the compiler could mistake it for a variable name, etc.
- The prefix increment operator is usually more efficient than the postfix one, since there is no need for temporary iterator copies.

Iterators

The properties of iterators depend on the underlying container:

array, vector, deque	Bidirectional (`++` / `--`), random access (i.e., instant jumps of arbitrary stride possible)
list	Bidirectional, no random access (must follow pointer chain)
forward_list	Forward direction only, neither backward direction nor random access
sorted assoc. cont.	See `list`
unsorted assoc. cont.	See `forward_list` [16]

The iterators provide their properties in the form of iterator tags (public members), which may be used to, e.g., write more efficient → template specializations of algorithms for iterators that provide random access.

[16] mainly because their order is arbitrary anyways

Algorithms

The Standard Library provides a large number of algorithms[17] that are tailored to these different iterator categories, and automatically make full use of the capabilities of the container they are operating on.

Example algorithms:

for_each	apply some function to each element (lifting)
count_if	count elements with certain properties
find_if	find first element with such property
copy_if	insert applicable elements into other container
shuffle	randomly re-order container contents
sort	sort container according to some criterion

Try to use predefined algorithms instead of writing your own function templates

[17] full list: https://en.cppreference.com/w/cpp/algorithm

Algorithms

Many of these algorithms expect some criterion, transform, or operation, which has to be supplied as a functor (function object): an object that has an `operator()` with the required number of arguments.

The Standard Library provides some default functors, e.g., `std::less`:

```
// possible implementation of std::less
template<typename T>
  struct less
  {
    // first set of () is operator name
    bool operator()(const T& lhs, const T& rhs) const
    {
      return lhs < rhs;
    }
  }
```

User-implemented functors can be used to customize the provided algorithms, or one can use → lambda expressions or function pointers instead.

Companion Classes

The Standard Library also provides a number of class templates that are not containers, but serve similar purposes as containers and are often used in conjunction with them.

`std::pair<T,U>`:

The official version of the `Pair` struct we defined ourselves. Contains a `T first` and a `U second`.

`std::tuple<T...>`:

Generalization of `std::pair` to general tuples using → variadic templates.

Member access through a `std::set` function, which expects either the type of the component as template parameter, or its index if the former is ambiguous.

C++17 adds → optional, → variant, and → any to the list.

Exceptions

C++ knows several different mechanisms for error handling:

`assert`:

Runtime check of some condition that should always be fulfilled (sanity check). Aborts the program if condition evaluates to `false`.

`static_assert`:

Compile-time check with similar purpose, see → template meta programming. Produces compilation error if condition is not met.

Exceptions:

Error handling mechanism for situations that should not be the norm, but may sporadically occur during normal operation: memory exhausted, file not found, matrix is singular, solver failed to converge...

Exceptions

An exception is an arbitrary object that can be interpreted as an alternative return value, delivered using a mechanism that differs from the standard `return`. The Standard Library provides some predefined exceptions for convenience, like `std::domain_error` and `std::range_error`, and new exceptions may be defined by inheriting from `std::exception`.

```
double nthroot(double x, int n)
{
  if (n % 2 == 0 && x < 0)
    // throw statement: execution of function is stopped here...
    throw std::domain_error("even powers require non-negative argument");

  ...
}

try // try block: register for treatment of potential exceptions
{
  double y = nthroot(-5.,2);
}
catch(std::domain_error e) // catch block: ...program control jumps here
{
  // try to do something better than just printing a message in practice
  std::cout << "nthroot failed, message: " << e.what() << std::endl;
}
```

Exceptions

Points to consider:

- Exceptions are for error conditions that can't be handled locally
- A `return` always returns to the immediate caller, but a `throw` unwinds the call stack until a matching `catch` block is found
- If none is found at all, the program is aborted (should be avoided if possible)
- All function calls between the `throw` statement and the `catch` block are stopped prematurely

This means that local resources have to be handled in those intermediate functions (allocated memory, open file handles, ongoing communication) during stack unwinding. An elegant mechanism to do this automatically is → RAII.

Advanced Topics

After having reviewed the basic building blocks of C++, i.e., the fundamental concepts and at least parts of the Standard Library, we discuss more advanced topics:

- template specializations
- interactions between templates and inheritance
- Resource Acquisition is Initialization (RAII)
- template metaprogramming
- dynamic polymorphism (virtual functions)
- static polymorphism (CRTP)
- Substitution Failure is not an Error (SFINAE)

Template Specialization

The main idea of templates is the reduction of code duplication through generalization, but sometimes there are special cases that should / have to be treated differently. This can be done by providing an explicit template specialization:

```
// make sure that int pointers are safe
template<> // empty set of remaining parameters
  struct Pair<int*> {int* a = nullptr; int* b = nullptr;};
```

For class templates[18], C++ additionally allows *partial* template specialization, where the template parameters are constrained but not fully specified:

```
// make sure pointers are safe
// note local change in meaning for U and V!
template<typename U, typename V>
  struct Pair<U*,V*> {U* a = nullptr; V* b = nullptr;};
```

Which version is chosen for a given instantiation, e.g., `Pair<int*,int*>` *?*

[18] and variable templates since C++14

Template Specialization

```
// 1) base template: general version
template<typename U, typename V = U>
  struct Pair;

// 2) partial specialization: U = V
template<typename U>
  struct Pair<U,U>;
// or shorter: Pair<U>

// 3) partial specialization: pointers
template<typename U, typename V>
  struct Pair<U*,V*>;

// 4) full specialization: int pointers
template<>
  struct Pair<int*,int*>;
// again, alternatively Pair<int*>
```

C++ always chooses the *most specialized* version:

- `Pair<int*,int*>` and `Pair<int*>` are (4), the latter via default argument in (1)
- `Pair<int,int>` and `Pair<int>` are both (2)
- `Pair<int*,double*>` is (3)

But `Pair<double*,double*>` and `Pair<double*>` are ambiguous, both (2) and (3) would fit!

Avoid overlapping specializations — they cause compiler errors when triggered

Template Specialization

Things are slightly more complicated for function templates. Assume for a moment that we have a function template for matrix-vector products:

```
template<typename Mat, typename Vec>
  Vec multiply(const Mat& mat, const Vec& vec);
```

If we had a class called `SparseMatrix` for sparse matrices, i.e., matrices where almost all entries are zero, this generic function would likely be very inefficient for such a matrix. It makes sense to provide a partial template specialization:

```
template<typename Vec>
  Vec multiply<SparseMatrix,Vec>
      (const SparseMatrix& mat, const Vec& vec);
```

Unfortunately, this isn't possible in C++.

Template Specialization

A full specialization would be allowed, and we could even omit the parameters:

```
template<>
  VectorClass multiply<SparseMatrix,VectorClass>
      (const SparseMatrix& mat, const VectorClass& vec);

// short version
template<>
  VectorClass multiply
  (const SparseMatrix& mat, const VectorClass& vec);
```

Alas, we would have to specialize for any of possibly many vector classes we would like to use together with `SparseMatrix`.

But why is that the case? Why can't we simply provide a partial specialization?

Dimov/Abrahams Example

Consider the following two code snippets[19]:

```
// (1) first base template
template<typename T> void f(T);

// (2) second base template (overloads)
template<typename T> void f(T*);

// (3) full specialization of (2)
template<> void f(int*);
```

```
// (1') first base template
template<typename T> void f(T);

// (3') full specialization of (1')!
template<> void f(int*);

// (2') second base template (overloads)
template<typename T> void f(T*);
```

(2) and (2') could be both a simple overload for, or a specialization of, (1) resp. (1'). In C++, the former is the case.

Now, consider the call `f(p)` for an `int* p`. This calls (3) as expected, but (2') for the second snippet[20]! *Why?*

Because in C++, overloads are resolved using base templates and normal functions, and *then* specializations are taken into account!

[19] see http://www.gotw.ca/publications/mill17.htm

[20] interactive version: link to godbolt.org

Dimov/Abrahams Example

As we have seen, even *full* function template specializations can lead to counterintuitive results, which may explain why partial ones are currently not part of the language.

This is a common issue with C++, where a newer feature (here: templates) has to take older ones (here: overloading) into account. The growth of C++ can be likened to onion layers, or strata of subsequent civilizations, and newer additions have to interact with well-established features.

This is also the reason why objects have an implicit self-reference pointer called `this`, and not a reference with that name: references were introduced after classes.

A particularly involved example we will consider throughout the lecture is compile-time template selection, which started with → SFINAE, is supported via → `enable_if` in C++11, → `enable_if_t` in C++14, and → `constexpr if` in C++17, and will be a standard application of → concepts in C++20.

Template Specialization (cont.)

Conclusions drawn from the aforementioned observations:

Class template specializations

These are perfectly fine, whether explicit (full) or partial specializations.

Function template specializations

Partial specializations are forbidden, use a helper class with partial specialization or incorporate the function as a method instead. Explicit specializations may interact in counterintuitive ways and are completely unnecessary: all types are fully specified, so simply provide a normal function overload instead.

"Use specializations for class templates, and overloads for function templates"

Template Specialization (cont.)

What about our motivating example, the sparse matrices?

We have the following options:

- Use overloading for one of the arguments, and templates for the other:

```
template<typename Vec>
  Vec multiply(const SparseMatrix& mat, const Vec& vec);
// + versions for each alternate matrix class
```

- Variant: make the `multiply` function a method for each of the matrix classes, maybe with some default that can be inherited from some base class.
- Hand computation over to some helper class template, which may freely use partial specialization:

```
template<typename Mat, typename Vec>
  Vec multiply(const Mat& mat, const Vec& vec)
  {
    return multHelper<Mat,Vec>::multiply(mat,vec);
  }
```

Classes and Templates: Interactions

The combination of object-oriented programming (inheritance) and generic programming (templates) leads to complications during name lookup that have to be studied in detail. C++ treats dependent and independent base classes in different ways.

Independent base classes are those base classes that are completely determined without considering template parameters, and independent names are unqualified names that don't depend on a template parameter.

- Independent base classes behave essentially like base classes in normal (non-template) classes.
- If a name appears in a class but no namespace precedes it (an unqualified name), then the compiler will look in the following order for a definition:
  1. Definitions in the class
  2. Definitions in independent base classes
  3. Template arguments
- This order of name lookup can lead to surprising results.

Classes and Templates: Interactions

```cpp
#include <iostream>

struct Base {typedef int T;};

template<typename T>
  struct Derived : Base
  {
    T val;
  };

int main()
{
  Derived<double> d;
  d.val = 2.5;
  std::cout << d.val << std::endl;
}
```

- This program prints `2`, not `2.5` as it may seem[a]
- `T` is not defined in the class, but in the independent base class
- Therefore, the template argument is ignored, and `T` is `int`! Main issue: this can't be seen when looking at `Derived`!
- Use different naming schemes for types and type placeholders (template parameters)

[a] link to godbolt.org

Classes and Templates: Interactions

Dependent base classes are those that are not independent, i.e., they require the specification of at least one template argument to be fully defined.

- The C++ standard dictates that independent names appearing in a template are resolved at their first occurrence.
- The strange behavior from the last example relied on the fact that independent base classes have higher priority during name lookup than template parameters.
- However, for names defined in a *dependent* base class, the resolution would depend on one or more template parameters, unknown at that point.
- This would have consequences when an *independent* name would have its definition in a *dependent* base class: it would have to be looked up before that is actually possible.

Classes and Templates: Interactions

```
template<typename T>
  struct Base {int n;};

template<typename T>
  struct Derived : public Base<T>
  {
    void f()
    {
      // (1) Would lead to type resolution
      //     and binding to int.
      n = 0;
    }
  };

template<>
  struct Base<bool>
  {
    // (2) Template specialization wants to
    //     define variable differently.
    enum {n = 42};
  };

void g(Derived<bool>& d)
{
  d.f();  // (3) Conflict
}
```

1. In the definition of class `Derived<T>`, the first access to `n` in `f()` would lead to binding `n` to `int` (because of the definition in the base class template).
2. Subsequently, however, the type of `n` would be modified into something unchangeable for the type `bool` as template parameter.
3. In the instantiation (3) a conflict would then occur.

Classes and Templates: Interactions

In order to prevent this situation, C++ defines that *independent* names won't be searched in *dependent* base classes. Base class attribute and method names must therefore be made dependent, so that they will only be resolved during instantiation (delayed type resolution).

Instead of simply writing `n = 0;`, use:

- `this->n = 0;` (implicitly dependent through `this` pointer)
- `Base<T>::n = 0;` (explicitly mentions template parameter)
- or import `n` into the current namespace:

```
template<typename T>
  struct Derived : Base<T>
  {
    // name is now dependent for whole class
    using Base<T>::n;
    ...
  };
```

Multiple Resource Allocation

Often, especially in constructors, resources must be allocated several times in succession (opening files, allocating memory, entering a lock in multithreading):

```
void useResources()
{
  // acquire resource r1
  ...
  // acquire resource r2
  ...
  // acquire resource rn
  ...
  // use r1...rn
  // release in reverse
  // release resource rn
  ...
  // release resource r1
  ...
}
```

- If acquiring `r_k` fails, `r_1,...,r_(k-1)` have to be released before cancellation is possible, otherwise a resource leak is created.
- What should be done if allocating the resource throws an exception that is caught outside? What happens to `r_1,...,r_(k-1)` ?

Multiple Resource Allocation

Common variant of this problem:

```
class X
{
  public:
    X();
    ~X();

  private:
    A* pointerA;
    B* pointerB;
    C* pointerC;
};
```

```
X::X()
{
  pointerA = new A;
  pointerB = new B;
  pointerC = new C;
}

// How can we guarantee that
// pointerA is freed if
// allocating pointerB or
// pointerC fails?
```

RAII

In C++, the correct solution for this problem is called "Resource Acquisition is Initialization" (RAII), which:

- is based on the properties of constructors and destructors and their interaction with exception handling.
- is actually a misnomer: "Destruction is Resource Release" (DIRR) would be more appropriate, but the acronym RAII is now too well-known to change it.

RAII is a specific way of thinking about resources that originated in C++ and provides an elegant alternative to strategies used in Java or Python, etc. (and has a really unfortunate name for something so central...).

RAII: Rules for Constructors and Destructors

Central rules that enable RAII:

1. An object is only fully constructed when its constructor is finished.
2. A compliant constructor tries to leave the system in a state with as few changes as possible if it can't be completed successfully.
3. If an object consists of sub-objects, then it is constructed as far as its parts are constructed.
4. If a scope (block, function...) is left, then the destructors of all successfully constructed objects are called.
5. An exception causes the program flow to exit all blocks between the `throw` and the corresponding `catch`.

The interplay of these rules, especially the last two, automatically frees resources before leaks can happen, even when unexpected errors occur.

Example Implementation

```
template<typename T>
  class Ptr
  {
    public:
      Ptr()
      {
        pointerT = new T;
      }

      ~Ptr()
      {
        delete pointerT;
      }

      T* operator->()
      {
        return pointerT;
      }

    private:
      T* pointerT;
  };
```

```
class X
{
  // no constructor and destructor
  // needed, the default variant
  // is sufficient
  private:
    Ptr<A> pointerA;
    Ptr<B> pointerB;
    Ptr<C> pointerC;
};

int main()
{
  try
  {
    X x;
  }
  catch (std::bad_alloc)
  {
    ...
  }
}
```

(This is actually a simple mock-up of → smart pointers)

Example Implementation

Basic principle:

- The constructor `X()` calls the constructors of `pointer{A,B,C}`.
- When an exception is thrown by the constructor of `pointerC`, then the destructors of `pointerA` and `pointerB` are called and the code in the `catch` block will be executed.
- This can be implemented in a similar fashion for the allocation of other resources (e.g. open files).

Main idea of RAII:

- Tie resources (e.g., on the heap) to handles (on the stack)[21], and let the scoping rules handle safe acquisition and release
- Repeat this recursively for resources of resources
- Let the special rules for exceptions and destructors handle partially-constructed objects

[21] heap: anonymous memory, freely allocatable; stack: automatic memory for local variables

Template Metaprogramming

Template metaprogramming refers to the use of templates to perform computations at compile-time. This comes in basically two flavors:

- Compute with numbers as usual, but during the compilation process
- "Compute" with types, i.e., automatically map some types to other types

The former precomputes results to speed up the execution of the finished program, while the latter is something that is impossible to achieve during runtime.

Template metaprogramming can't make use of loops and is therefore inherently recursive when performing nontrivial computations, and may become arbitrarily complex (it is Turing complete!). We will only look at some small introductory examples.

→ SFINAE can be seen as a special case of template metaprogramming.
→ Constant expressions can often serve as a modern replacement for template metaprogramming, especially since loops in `constexpr` functions have been added in C++14.

Compile-Time Computations

An example of compile time single recursion to compute the factorial:

```
template<int N>
  struct Factorial
  {
    enum {value = Factorial<N-1>::value * N};
  };

// base case to break infinite recursion
template<>
  struct Factorial<0>
  {
    enum {value = 1};
  };
```

In modern C++, this can be simplified significantly using → variable templates, because one doesn't need enums or static attributes for the values anymore.

Recursive Type Construction

Automated type generation using template metaprogramming:

```
template<typename T, int N>
  struct Array : public Array<T, N-1>
  {
    template<int M>
      T& entry()
      {
        return Array<T, M+1>::val;
      }

    // hide implementation detail
    protected:
      T val;
  };

// empty base case
template<typename T>
  struct Array<T,0>
  {};

// use like this:
Array<double,3> a;
a.entry<0>() = 0;
a.entry<1>() = 1;
a.entry<2>() = 2;
```

- Recursive definition: array of N elements is array of $N-1$ elements plus additional value
- Helper method for element access
- Nice feature: going beyond array bounds triggers compilation error
- Storing different types as in `std::tuple` would require → variadic templates and be significantly less straight-forward to implement
- Also see `dune-typetree`, a library for compile-time construction and traversal of tree structures[a]

[a] Link: gitlab.dune-project.org/staging/dune-typetree

Dynamic Polymorphism

Inheritance is based on new code utilizing old code: we augment an existing class with new data/methods, and these can make use of the interface and/or implementation of the base class.

The main idea behind dynamic polymorphism (subtyping) is trying to make the inverse work: have old code utilize new code, i.e., we want to inject new behavior into classes and function without modifications to existing code.

Here, the concept polymorphism (greek: "many forms") refers to several functions sharing a common interface, with the concrete variant that is chosen depending on the provided arguments. The desired injection of new behavior is achieved by making this selection independent of the function call site.

Types of Polymorphism

There are different types of polymorphism:

- Static polymorphism, with the function being chosen at compile-time:
  - Ad-hoc polymorphism, in the form of function and operator overloading
  - Parametric polymorphism, in the form of templates and specializations
  - "True" → static polymorphism, trying to emulate dynamic polymorphism using template metaprogramming

  Also known as early binding, i.e., during program creation.
- Dynamic polymorphism, with the function being chosen at runtime (also known as late binding).

In C++, static polymorphism is multiple dispatch (the combination of types determines the chosen variant), while dynamic polymorphism is always single dispatch[22] (only depends on the object itself, not the method arguments).

[22] Dynamic multiple dispatch exists, e.g., in the Julia language.

Slicing

Using the copy constructor or assignment operator of a base class on some object results in slicing: anything belonging to the derived class is cut away, and only the base class part is used in the assignment.

Something similar happens when a base class pointer or base class reference referring to an object of the derived class is created: only the base class methods and attributes are accessible through such pointers and references. If the derived class redefines certain methods, then the base class version is used anyways, i.e., the pointer/reference type dictates behavior, not the type of the object itself.

Polymorphic Types

Polymorphic types are classes that have at least one method defined as `virtual`. For such methods, the type of the object itself determines which version is actually called, not the type of references or pointers:

```
struct Base
{
  virtual void foo() {...};
};

struct Derived : public Base
{
  void foo() override {...};
}

Derived d;
Base& b = d;
b.foo(); // calls foo() of Derived
```

Polymorphic Types

- In C++, methods have to be explicitly declared as `virtual` for this to work. In some other languages this behavior is actually the default, e.g., in Java.
- There is no reason to (re-)declare the same method as `virtual` in derived classes, this happens automatically. But one may use `override` to state that this method should override a base class method, and will get a compilation error if this doesn't actually happen.
- Without the `override` qualifier the compiler would silently introduce an overload if the signature doesn't match, and consequently the base class method might be called when that isn't expected to happen.

Implementation Detail: vtables

Using polymorphic types, i.e., virtual functions, incurs a certain runtime cost: the concrete version to use for a certain function call has to be decided at runtime, because it depends on the actual type of the object pointed / referred to (that's the whole point).

A standard way of implementing virtual functions is via vtables (dispatch tables):

- Each class with at least one virtual method stores hidden static tables of virtual functions ("vtables"), one for each base class with virtual methods, and potentially one for the class itself.
- These tables contain function pointers to the right method versions.
- Each object of such a class contains hidden pointers to the relevant vtables.
- These are inherited from the base class and therefore remain after slicing, etc., but are redefined to point to the local version of the tables.

Implementation Detail: vtables

```
struct Base1
{
  // creates entry in vtable
  virtual void foo1();
}

struct Base2
{
  // creates entry in vtable
  virtual void foo2();
}

struct Derived : Base1, Base2
{
  // changes entry in vtable
  void foo2() override;
  // creates entry in vtable
  virtual void bar;
}

Derived d;
Base2& b2 = d;
// follow two pointers for call here
// (p. to table and p. to function)
b2.foo2();
```

- The class `Derived` contains three implicitly defined static tables, one for itself, and one for the two base classes each.
- The table from `Base1` is copied, but that of `Base2` is changed locally, with its entry pointing to `Derived::foo2` instead.
- The call `b2.foo2()` accesses the vtable through the hidden pointer, and then uses the function pointer to `Derived::foo2` it finds there.
- Cost for lookup: follow two pointers (relevant when the method is very simple and called very often)

Virtual Destructors

Polymorphic types can be stored in containers and similar classes via pointers to base classes, and retain their specialized behavior. This makes it possible to use containers for heterogeneous collections of objects, as long as they all have a common base class.

However, the container would trigger the destructor of the base class when it goes out of scope, not the destructors of the derived classes. For this reason it is common practice to declare a public virtual destructor when at least one other virtual method is present, to ensure that the destructors of the derived classes are called.

Note that this suppresses the automatic generation of copy/move constructors and operators, but normally directly copying polymorphic types isn't a good idea anyways.

Copying Polymorphic Types

If a polymorphic object is copied when accessed through a base class pointer, the base class constructor is used. This means that unintended slicing occurs: only the base class part is copied, and virtual method calls revert back to the version of the base class.

The desired behavior would usually be a full copy of the object, i.e., based on its true type and consistent with dynamic polymorphism. This would require something like a "virtual constructor" that constructs the correct type. But constructors can't be virtual, because they are not tied to objects — they are part of the class itself, like static methods.

The standard solution to this problem is:

- explicitly forbid copying (and moving) polymorphic objects
- provide a special clone method, that serves the purpose of such virtual constructors, but operates on the level of pointers

Copying Polymorphic Types

```
class Base
{
  // define copy/move constructors
  // and operators here

  public:
    virtual Base* clone() const
    {
      return new Base(*this);
    }

    // virtual destructor
    virtual ~Base() {}
};

class Derived : public Base
{
  // as above

  public:
    Derived* clone() const override
    {
      return new Derived(*this);
    }
};
```

- Calling the `clone` method on a `Base` pointer will create a copy of the correct type and return a pointer to it.
- Using covariant return types (see LSP) we may return a pointer to the actual type.
- This pattern doesn't follow RAII at all. This can be changed using → smart pointers, but then a pointer to the base class has to be used throughout, since smart pointers of covariant types are not themselves covariant.

Abstract Base Classes

Abstract base classes (ABCs) are base classes that have at least one method declared as purely virtual, i.e., declared as a virtual function, but without actually providing a default implementation:

```
struct ABC
{
  virtual void foo() = 0; // pure virtual: no definition provided
  virtual ~ABC() {} // virtual destructor
};
```

Abstract base classes are used to define interfaces, because of the following two properties:

- It is impossible to instantiate objects of such a class, because at least one method is missing a definition.
- Every derived class has to provide such a definition to become instantiable.

Example from DUNE

```
template<class X, class Y>
class Preconditioner {
  public:
    //! \brief The domain type of the preconditioner.
    typedef X domain_type;
    //! \brief The range type of the preconditioner.
    typedef Y range_type;
    //! \brief The field type of the preconditioner.
    typedef typename X::field_type field_type;

    //! \brief Prepare the preconditioner. (...)
    virtual void pre (X& x, Y& b) = 0;

    //! \brief Apply one step of the preconditioner (...)
    virtual void apply (X& v, const Y& d) = 0;

    //! \brief Clean up.
    virtual void post (X& x) = 0;

    ...

    //! every abstract base class has a virtual destructor
    virtual ~Preconditioner () {}
};
```

Abstract base class for preconditioners:

- defines some types
- declares some methods, but doesn't provide implementations
- includes virtual destructor

Multiple Inheritance

Multiple interfaces can be combined by inheriting from several ABCs:

```
// VectorInterface: interface for vector types
// FunctionInterface: interface for functors
class Polynomial : public VectorInterface, FunctionInterface
{
  // define any methods required by the ABCs
}
```

`VectorInterface` might define (but not implement) all the usual methods for vector arithmetics, while `FunctionInterface` would require an appropriate `operator()`.

In the above code example, `FunctionInterface` is not a template, and therefore would describe the usual functions of a single real variable, but it wouldn't be difficult to provide a class template as ABC instead. This would also cover more general functions (and technically define a parameterized family of ABCs).

Multiple Inheritance

Multiple inheritance is simple for ABCs, because they typically don't contain data. Therefore, the interface conditions are simply restated, i.e., this form of multiple inheritance is perfectly fine.

Multiple inheritance of base classes containing data, however, may lead to duplication of data members. To avoid this, virtual inheritance can be used: the derived class contains one copy of the base class per non-virtual derivation, and a single one for all virtual derivations combined.

This diamond pattern, sometimes called Deadly Diamond of Death, typically leads to code that is hard to maintain and may contain subtle bugs:

- Forgetting one of the `virtual` specifiers silently creates a second copy of the base class data.
- Accessing the data in this second unmaintained version by accident will make the state of the derived object inconsistent.

Example from DUNE

In practice, the diamond pattern is discouraged because of the resulting high maintenance cost. However, earlier versions of PDELab contained a Newton method based on this pattern that may serve as demonstration.

A Newton method consists of:

- a basic algorithm
- steps that must be performed at the start of each Newton iteration (e.g. reassembly of the Jacobi matrix)
- a test whether the process has converged
- optionally a linesearch to enlarge the convergence area

Each of these intermediate steps is outsourced to a separate class, so you can replace all the components independently.

The common data and virtual methods are placed in a base class.

Example from DUNE

```
// data to operate on, iteration count, etc.
class NewtonBase
{...};

// perform linear solve, compute step direction
class NewtonSolver : public virtual NewtonBase
{...};

// check termination criterion
class NewtonTerminate : public virtual NewtonBase
{...};

// perform line search strategy
class NewtonLineSearch : public virtual NewtonBase
{...};

// local linearization (jacobian), thresholds, etc.
class NewtonPrepareStep : public virtual NewtonBase
{...};

// combine above classes into one complete class
class Newton : public NewtonSolver, public NewtonTerminate,
               public NewtonLineSearch, public NewtonPrepareStep
{...};
```

The actual implementation combined this with templatization on all levels.

Static Polymorphism

Just as dynamic polymorphism refers to the ability of code to adapt to its context *at runtime*, with dynamic dispatch on the type of objects, static polymorphism refers to polymorphism at compile-time with similar goals.

We have already discussed two versions of such static polymorphism:

- function and operator overloading
- templates and their specializations

Older code may then be adapted to new types by adhering to the relevant interfaces. But there is also a specific pattern for static polymorphism that mimics virtual function calls, but resolved at compile-time: base class templates using the curiously recurring template pattern.

Static Polymorphism

In the Curiously Recurring Template Pattern (CRTP), some class is used as a template parameter of its own base class. This is actually valid C++, because the full definition of the derived class isn't required at that point, only during instantiation.

```
template<typename T>
  class Base
  {
    // access to members of T through template parameter
    ...
  };

class Derived : public Base<Derived>
{
  ...
};
```

Also sometimes called Upside-Down Inheritance, because class hierarchies can be extended through different base classes using specialization.

Static Polymorphism

```
template<typename T>
  struct Base
  { // base class: provide interface, call impl.
    static void static_interface()
    {
      T::static_implementation();
    }
    void interface()
    {
      static_cast<T*>(this)->implementation();
    }
  };

struct Derived : public Base<Derived>
{ // derived class: provide implementation
  static void static_implementation();
  void implementation();
}

// call this with Derived object as argument
template<typename T>
  void foo(Base<T>& base)
  {
    Base<T>::static_interface();
    base.interface();
  }
```

- `static_cast` converts pointer types at compile-time, is type-safe (i.e., only works if `Base` object is actually part of a `T` object)
- Base class provides interface definition like in ABCs
- Avoids cost of virtual functions
- Not a full replacement for dynamic polymorphism, e.g., no common base class as needed for STL containers

Example from DUNE

Mixin to define finite element Jacobian in terms of residual evaluations, with `Imp` being both template parameter and derived class:

```
template<typename Imp>
class NumericalJacobianVolume
{
public:
  ...

   //! compute local jacobian of the volume term
   template<typename EG, typename LFSU, typename X, typename LFSV, typename Jacobian>
   void jacobian_volume (const EG& eg, const LFSU& lfsu, const X& x,
                         const LFSV& lfsv, Jacobian& mat) const
   {
     ...
     asImp().alpha_volume(eg,lfsu,u,lfsv,downview);
     ...
   }

private:
  const double epsilon; // problem: this depends on data type R!
  Imp& asImp () { return static_cast<Imp &> (*this); }
  const Imp& asImp () const { return static_cast<const Imp &>(*this); }
};
```

SFINAE

We have already discussed how the compiler chooses between several available template specializations: it picks the "most specialized" version for which the template parameters lead to successful instantiation.

During this selection process, other (more specialized) versions may have to be tried out, but ultimately rejected when substituting the parameters with the given types fails. Therefore:

"Substitution Failure is not an Error" (SFINAE)

Failing to instantiate one of the specializations doesn't terminate the compilation process, that happens only when the pool of possible choices has been exhausted and no viable specialization was found, or several that are equally suitable.

SFINAE

SFINAE, the programming technique with the same name, provides a mechanism to select between different template specializations at will, and achieves this by triggering substitution failures on purpose.

The main tool for this is a small template metaprogram named `enable_if`, which provides a type definition or doesn't, depending on some external condition:

```
// possible implementation of enable_if
// ``false case'' --> no dependent type defined
template<bool B, class T = void>
  struct enable_if {};

// ``true case''  --> dependent type is defined
template<class T>
  struct enable_if<true, T> {typedef T type;};
```

Picking Numerical Solvers

Assume we have a set of numerical problems, say, `ProblemA`, `ProblemB`, and maybe others, and also a set of solvers for such problems, `Solver1`, `Solver2`, and potentially some others. We decide to manage the different combinations using a common interface:

```
template<typename Problem,
         typename Solver = Problem::DefaultSolver>
  void solve(...)
  {
    // instantiate Problem and configure it
    // instantiate appropriate Solver
    // apply Solver to Problem
    // postprocessing, etc.
  }
```

This works fine as long as every problem class defines an appropriate solver default.

Picking Numerical Solvers

There are two points to consider:

- The default solver is only a suggestion and another one may be chosen by the user. This includes solvers that compile fine but are maybe not numerically stable for the given problem!
- Maybe we want to eliminate the `Solver` template parameter altogether, instead automatically choosing a suitable solver from our collection for any problem that is passed to the `solve` function.

For this to work, we have let our different `solve` variants know about certain "properties" of the problem classes, and maybe also of the solver classes. These can then be used to mask those combinations we don't want to be used via SFINAE.

Solving Linear Systems

To discuss a smaller application in more detail and show how SFINAE is actually used, let us assume we have several matrix classes available, and some of them provide a method named `multiplyWithInverse` that solves

$$Ax = b$$

in a very specialized and efficient way[23], and others don't. We want to make use of this functionality when it is available, of course, i.e., we have to check whether the method exists.

We need the following ingredients:

- A traits class template that checks for the existance of the above method
- The aforementioned `enable_if` to potentially define a type, depending on the "return value" of the traits class
- Different `solve` functions, picking the right one with SFINAE

[23] e.g., some precomputed matrix decomposition, a specialized spectral method, etc.

Solving Linear Systems

Traits class for existance of method, adapted from Jean Guegant's example[24]:

```
template <class T1, class T2>
  struct hasMultiplyWithInverse
  {
    // Truth values at compile time
    typedef struct{char a; char b;} yes; // size 2
    typedef struct{char a;}         no;  // size 1

    // Helper template declaration
    template <typename U, U u> struct isMethod;

    // Picked if helper template declares valid type, i.e. if signature matches:
    // - const C1 as implicit first argument to method [(C1::*) ... const]
    // - non-const reference to C2 as second argument, and void as return type
    template <typename C1, typename C2>
      static yes test(isMethod<void (C1::*)(C2&) const, &C1::multiplyWithInverse>*) {}

    // Catch-all default (templatized C-style variadic function)
    template <typename,typename> static no test(...) {}

    // Export truth value (as enum, alternatively as static const bool)
    // Trick: sizeof works without actually calling the function
    enum {value = (sizeof(test<T1,T2>(0)) == sizeof(yes))};
  };
```

[24] https://jguegant.github.io/blogs/tech/sfinae-introduction.html

Solving Linear Systems

Two versions of the `solve` function, one of them being selected by SFINAE:

```
template<typename M, typename V>
  typename std::enable_if<hasMultiplyWithInverse<M,V>::value>::type
  solve(const M& m, V& v)
  {
    // implement specialized version here, can use multiplyWithInverse
  }

template<typename M, typename V>
  typename std::enable_if<!hasMultiplyWithInverse<M,V>::value>::type
  solve(const M& m, V& v)
  {
    // implement general version here, has to avoid multiplyWithInverse
  }
```

Standard placements of `enable_if`:

- Additional template parameter, hidden by assigning default value
- Additional function argument, hidden by assigning default value
- Return type of function (chosen above)

SFINAE (cont.)

Central steps to make this form of SFINAE work:

- Use template specialization to determine at compile time whether some type has a certain method or not
- Use this inside `enable_if` to trigger substitution failures on purpose
- Guide compiler to select correct specialization (i.e., remove ambiguity)

The SFINAE code presented above is valid C++98/03. C++11 and later standards introduced several features that make SFINAE significantly simpler, or help avoid it altogether:

- → Constant expressions, e.g., to avoid the `sizeof` trick/hack
- Predefined → type traits, to simplify writing conditionals
- Mapping between values and their types (→ decltype/declval)

SFINAE (cont.)

A simplified version based on C++11, extracting type information using decltype:

```
template<typename T1, typename T2>
  struct hasMultiplyWithInverse
  {
    template<typename T, typename U = void> // (1)
      struct Helper
      {enum {value = false};};

    template<typename T>                    // (2)
      struct Helper<T,decltype(&T::multiplyWithInverse)>
      {enum {value = true};};

    // matches (2) if function exists, else matches (1)
    enum {value = Helper<T1,void (T1::*)(T2&) const>::value};
  };
```

Example from DUNE

The product of two functions on a numerical grid can be defined if

- both have the same dimensionality (i.e., scalar product of vector fields)
- or one of them is a scalar function (i.e., simple scaling)

Base template, handling the first case (also an example of CRTP):

```
//! Product of two GridFunctions
template<typename GF1, typename GF2, class = void>
class ProductGridFunctionAdapter :
  public GridFunctionBase<
    GridFunctionTraits<
      typename GF1::Traits::GridViewType,
      typename GF1::Traits::RangeFieldType, 1,
      FieldVector<typename GF1::Traits::RangeFieldType, 1> >,
    ProductGridFunctionAdapter<GF1,GF2> >
{
  static_assert(unsigned(GF1::Traits::dimRange) ==
                unsigned(GF2::Traits::dimRange),
                "ProductGridFunctionAdapter: Operands must have "
                "matching range dimensions, or one operand must be "
                "scalar-valued.");
  ...
};
```

Example from DUNE

Specializations for the two different semi-scalar cases, using SFINAE:

```
//! Product of two GridFunctions
template<typename GF1, typename GF2>
class ProductGridFunctionAdapter<GF1, GF2,
  typename std::enable_if<
    GF1::Traits::dimRange == 1 && GF2::Traits::dimRange != 1
    >::type> :
  public GridFunctionBase<typename GF2::Traits, ProductGridFunctionAdapter<GF1,GF2> >
{
  ...
};

//! Product of two GridFunctions
template<typename GF1, typename GF2>
class ProductGridFunctionAdapter<GF1, GF2,
  typename std::enable_if<
    GF1::Traits::dimRange != 1 && GF2::Traits::dimRange == 1
    >::type> :
  public ProductGridFunctionAdapter<GF2, GF1>
{
public:
  ProductGridFunctionAdapter(GF1& gf1, GF2& gf2)
    : ProductGridFunctionAdapter<GF2, GF1>(gf2, gf1)
  { }
};
```