Programming Techniques for Scientific Simulations

1 IMPORTANT

» C++: `const` whenever possible!
» Python: don't forget docstring and `self` in non-static member functions

2 Table of contents

3 Git

.gitignore

```
#Ignore all
*
#Unignore all with extensions
!*.*
#Unignore all dirs
!*/
#Result: Ignore only binaries (no extension)
```

Setup:

```
git config -global user.name "Robin"
git config -global user.email "a@b.c"
```

Commands: init, fetch, status, log, help, add, commit, push, pull, branch, checkout, merge

4 Unix Shell

» Move/copy: `mv/cp source/file.c dest/file.c`
» Copy directory: `cp -r <src> <dest>`
» Rename: `mv ./asdf.txt ./qwer.txt`
» Remove: `rm (-r) <path>`

» Redirect output: `wc -l *.txt > out.txt`
» Sort & append: `sort -n out.txt >> out.txt`
» Input from file:

```
./main < input.txt
./main < <(echo 1 2 3)
echo 1 2 3 | ./main
```

Pipe: Combine multiple commands

```
wc -l *.txt | sort -n | head -n 1
ls | grep "test" | tail -n 2
```

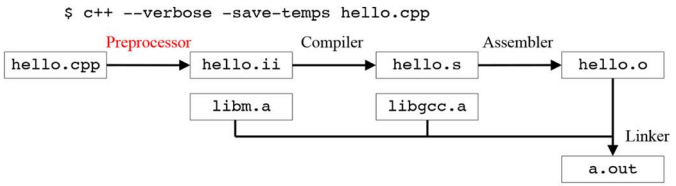
Wildcard: `*` = zero or more chars; `?` = 1 character

Tools:
» `wc <file>`: #lines #words #chars (`-l` only #lines)
» `sort <file>` (default alphanum., `-n` for numerical, `-r` reverse)
» `cat / less`: print content of file
» `echo`: print argument
» `cut`: cut out sections of each line (e.g. text before ",")

```
cut -d , -f 1 test.txt
```

Robin, 19 ⇒ Robin

5 Compiling & Linking



Run until: Preprocessor (-E), Compiler (-S), Assembler (binary) (-c)

Compile multiple files separately, link afterwards
Compile the file `square.cpp`, with the `-c` option (no linking)

```
$ c++ -c square.cpp
```

Compile the file `main.cpp`, with the `-c` option (no linking)

```
$ c++ -c main.cpp
```

Link the object files

```
$ c++ main.o square.o
```

Link the object files and name it, e.g `square`

```
$ c++ main.o square.o -o square
```

Include guards (for header files)

```
#ifndef HEADER_HPP
#define HEADER_HPP
// declarations
#endif /* HEADER_HPP */
```

6 Libraries

» Static libraries: `lib*.a`
  » At link time, only the used functions from the archive are copied into the executable
  » Compile the sources into object files
  `g++ -c square.cpp`
  » Pack the object files into a static library
  `ar -crs libsquare.a square.o`
  » Name must be `lib`something`.a`
» Shared libraries: `lib*.so`
  » The functions from the library are not copied into the executable. Instead, the library is loaded only once into memory where it can be used by any executable.
  » Compile the sources into Position Independent Code (PIC) object files
  `g++ -fPIC -c square.cpp`
  » Pack the object files into a shared library
  `g++ -shared -fPIC -o libsquare.so square.o`

» The name must be `libsomething.so`

» Use libraries

» Compile the main (include path to library!)
`g++ -c -I lib main.cpp`

» Link the object files
`g++ -o main main.o -Llib -lsquare`

» `-L` + folder of library, `-l` + name of library

» Order of libraries is important! If `libA.a` calls a function in `libB.a`, you need to link in the right order: `-lA -lB`

» cf. Demo Week 2 / Ex. 2-2

Document library with: Signature of functions, semantics, pre-/post-conditions, dependencies, exception guarantees, references

7 Make & CMake

Make

» `make` (runs Makefile) or run `make -f make.mk` (builds first target by default). `make -n` just prints commands (useful for debugging)

» Define targets with dependencies/prerequisites

```
target: prerequisites
[TAB] commands
```

» Use this struct to build all

```
-include config.mk
.PHONY: all
all: square
```

» `config.mk` defines compiler version, flags etc.; should not go under version control / be pushed if personal paths are used.

» Variables

`$@`	file name of the target of the rule
`$<`	name of the first prerequisite
`$^`	names of all the prerequisites, separated by space
`CC`	program for compiling C progs; def. cc
`CXX`	program for compiling C++ progs; def. g++
`RM`	command to remove a file; def "rm -f"
`CFLAGS`	extra flags for C compiler
`CXXFLAGS`	extra flags for C++ compiler
`LDFLAGS`	extra flags for compiler when linking
`LDLIBS`	library flags/names for compilers when linking

```
square.o: square.cpp square.hpp
	${CXX} ${CXXFLAGS} $<
main.o: main.cpp square.hpp
	${CXX} ${CXXFLAGS} $<
square: main.o square.o
	${CXX} ${CXXFLAGS} -o $@ $^
```

» Cleaning

```
.PHONY clean
clean:
	${RM} -v *.o square
```

» cf. Demo Week 2 (square/square lib) / Ex. 2-2 / 2-3

CMake

» cross-platform build system generator

» Create `CMakeLists.txt` in source directory

» `cd <build-dir>; cmake <src-dir>`

» Use `ccmake <src-dir>` to specify settings, compiler flags, etc.

» cf. Ex 3-1 / Demo Week 3

» Useful functions

» `project()` set project name, useful for debugging

» `add_executable(<target name> <src files>)` compile an executable

» `add_library(<name> <type> <src files>)` create lib (SHARED/STATIC)

» `target_link_libraries(<target> <libs>)` makes lib accessible to the target, adds it in linking process

» `add_subdirectory(<path>)` run CMakeLists in a subdirectory, e.g. for library

» `include_directories(<path>)` tell preprocessor where to look for files to include

» cf. Ex 06 / Penna on how to use subdirectories.

8 Generic Programming

» If functions are **overloaded**, the compiler chooses the best fit.

» No type safety when using **macros** + unexpected side effects

```
#define MIN(x, y) (x < y ? x : y)
MIN(x++, y++); // smaller number incremented twice!
⇒ (x++ < y++ ? x++ : y++)
```

» **Templated** version: Usage causes instatiation. Type safe, compile error if misused.

```
template <typename T>
T min(T x, T y) {
  return (x < y ? x : y); }
int min(int x, int y); // if called with int args
double min(double x, double y); // with double args
```

Requirements on `T`? `operator<` with result convertible to bool; Copyable (pass by value), not needed if changed to `const T&`

» **Definition Polymorphism**: Using many different types through the same interface

» Documenting a function template: Pre-/Postconditions, semantics, exception guarantees. New: concept requirements on types.

» **Complete source code of the template function must be in a header file**

» Specialize a templated function/struct etc.

```
template<typename T>
struct helper { typedef T type; };
template<>
struct helper<int> {typedef double type; };
```

Type Traits

» "Calculate" which type should be used in the template e.g. when adding two vectors of different types

» Examples slide 05b.6f.

» **Concept**: Set of requirements on types

» The operations the type must provide

» Their semantics (meaning of the operations)

» Their time/space complexity

» Concept defined by C standard. E.g. *regular type*

» CopyConstructible

» Assignable

» EqualityComparable

» Destructible

» cf. Demo Week 5 (Traits)

9 Data structures

Classes

» public: only representation-independent interface, accessible to all

» private: representation-dependent functions and data members

» friend: declarators allow related function/classes access to representation

» Default constructor = constructor without arguments

» Constructor: Order of member initialization: same as declaration in class. Sometimes initializer list is necessary: No other way of setting members that are const, reference or of a class type without default ctor. **No `const` members if class should be copy-assignable!**

» Use `typedef` to define recurring types (`typedef double coord_t;`) or `using` (`using coord_t = double;`)

» `mutable` keyword allows member variable to change value through a `const` member function

```cpp
class A {
  public:
    int func() const;
  private:
    mutable int cnt_;
};
int A::func() const {
  cnt_++; // OK!
  return 42;
}
```

» **`static`** member: one variable for all objects of the same class, e.g. a count/id. Must be initialized. Exist even without an object, thus access via scope operator (`::`)

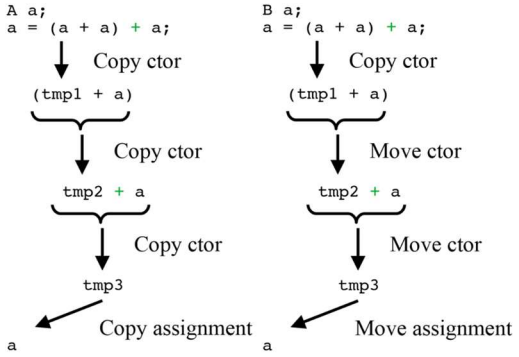
» **`friend`** grants a function or another class access to the private and protected members of the class

» Special member functions

```cpp
T();                    // default ctor
~T();                   // dtor
T(const T&);            // copy ctor
T& operator=(const T&); // copy assignment
T(T&&);                 // move ctor
T& operator=(T&&);      // move assignment
```

Move ctor/assignment moves a temporary object into the new/another object. Acts on rvalue references/xvalues.

» Copying vs. moving



» Rule of three: dtor, copy ctor + assignment

» Rule of five: dtor, copy ctor + assignment, move ctor + assignment

» std::move produces an xvalue expression.

```cpp
std::move(first, last, first_new); // moves [first, last[ to first_new
T a = T(std::move(b)); // move ctor
```

» cf. Demos Week 5 (SArray) for implementation details (SArrayT for templated version)

» cf. Ex. 7-1 Iterators

» Some operators might need to be written twice, with and without `const`

Static Variables

Variables persist through the whole program and are not deleted at the end of scope

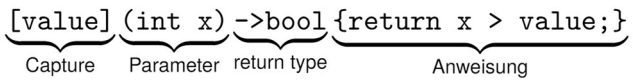
```cpp
// function example
void foo() {
 //only executed the first time
 static int count = 0;
 //executed every time, value persists
 count++;
}
// loop example
for(int i = 0; i < 5; ++i) {
 static int count = 0;
 count++;
}
```

Funktoren

» Struct/Class, deren `operator()` überladen ist.

» Funktionen, die aber auch einen Zustand annehmen können.

» **Lambda-Expressions** sind Inline-Funktoren/anonyme Fkt.



» Return type und Parameter können weggelassen werden

» Minimale Lambda-Expression: `[]{}` (Aufruf: `[]{}();`)

» Verschiedene Captures

» `[x]`: Zugriff auf kopierten Wert von x (nur lesend)

» `[&x]`: Zugriff auf Referenz von x

» `[&x, y]`: Zugriff auf Ref. x und Wert von y

» `[&]`: Default-Referenz-Zugriff auf alle Objekte im Kontext der Lambda-Expression

» `[=]`: Default-Werte-Zugriff auf alle Objekte im Kontext der Lambda-Expression.

» Achtung bei Funktoren innerhalb von Klassen

```cpp
struct mutant {
 int i = 0;
 void do(){ [=]{i = 1;}(); } };
mutant m; m.do();
cout << m.i; // 1, weil bei der λ-Expr. der this-Pointer (this->i) implizit kopiert wird, nicht die Variable selbst.
```

» cf. Ex. 5-2 Simpson2D (nested Lambdas)

Smart Pointers

```cpp
std::shared_ptr<int> p = std::make_shared<int>(3);
```

Operator overloading

Expression	Operator	Member function	Non-member function
`@a`	`+ - * & ! ~ ++ --`	`A::operator@()`	`operator@(A)`
`a@`	`++ --`	`A::operator@(int)`	`operator@(A,int)`
`a@b`	`+ - * / % ^ & | < > == != <= >= << >> && || ,`	`A::operator@(B)`	`operator@(A,B)`
`a@b`	`= += -= *= /= %= ^= &= |= <<= >>= []`	`A::operator@(B)`	-
`a(b,c...)`	`()`	`A::operator()(B,C...)`	-
`a->b`	`->`	`A::operator->()`	-
`(TYPE) a`	`TYPE`	`A::operator TYPE()`	-

Polymorphism

Access	public	protected	private
Members of the same class	yes	yes	yes
Members of derived class	yes	yes	no
Not members	yes	no	no

» The derived class inherits all members of the base class except: ctors, dtor, assignment operators, friends, private members.

» **Virtual functions**: Can be redefined in a derived class while preserving its interface and get correctly redirected to the derived class when called through a base class pointer/reference.

» Classes that declare or inherit virtual functions are called polymorphic classes.

» **Abstract Base Class (ABC)** is a class that contains one (or more) pure virtual functions. Pure virtual functions are functions without a definition in the base class. We are declaring an interface that all derived classes must adhere! ABC's cannot be used to instantiate objects.

» Use `override` keyword to make sure that the function is virtual and is overriding a virtual function from a base class (inheritance05.cpp).

» Use `final` keyword to make sure that the function cannot be overridden by derived classes

Runtime polymorphism	Compile time polymorphism
Use virtual functions	Use templates
Decision at runtime	Decision at compile time
Works for objects derived from the common base	Works for objects having the right members (concepts)
One function created for the base class → saves space	A new function created for each class used → more space

Virtual function call needs lookup in type table → slower	No virtual function call, can be inlined → faster
Extension possible using only definition of base class	Extension needs definition and implementations of all functions
Most useful for application frameworks, user interfaces, big functions	Useful for small, low-level constructs, small fast functions, generic algorithms

10 Exceptions

» Exception is an object of any type
» Thrown using the throw keyword

```
if(n <= 0) throw "n too small"; // throw char[]
if(index >= size) throw std::range_error("index");
```

» Std. exceptions from `<stdexcept>`, derived from `std::exception`
» `std::logic_error`
  » domain_error: value outside domain of variable
  » invalid_argument: argument is invalid
  » length_error: size too big
  » out_of_range: argument has invalid value
» `std::runtime_error`
  » range_error: invalid value occurred as part of calculation
  » overflow_error: value got too large
  » underflow_error: value got too small
» Specifier `noexcept`: compiler know that the function will never throw an exception (e.g. destructors should never fail).
» cf. Demo Week 6

11 Optimizing, Timing & Profiling

Optimizations

» Most important: Use compiler optimizations. (-O0, ..., O5, Os (size)), use `-fopt-info` to see optimization reports
» Use different algorithm/data structure for lower asymptotic runtime
» Use Assembly instructions. Code becomes non-portable!
» Between asm and C++: Compiler intrinsics
  » Many compilers support a long list of intrinsic functions that look like functions but get mapped directly to assembly statements.
  » Needs special compiler flag
  » cf. Demo Week 10
» Change associativity (e.g. of matrices), can be done by compiler in simple cases or precompute certain things.
» Minimize work done in loops.
» Dead code removal: Compiler detects if a statement is never executed.
» Keep storage order in mind (row-/col-major, strides)

C++ specific optimizations

» C++ compiler with templates is a Turing machine
» **Template Metaprogramming (TMP)**: Perform loops (recursion) and do branches at compile time
» cf. Demo Week 11 for examples (dot product & Unruh (primes))
» **Expression templates** (ET). Example:

```
a = b + c + d;
for(int i = 0; i < a.size(); ++i)
  a[i] = b[i] + c[i] + d[i];
```

» Lazy evaluation: Postpone evaluation of an expression until assignment. Don't evaluate temporary terms of a computation.
» cf. Demo Week 11 (etvector)

Timing

» C++: `<chrono>` but use simple timer library
  » cf. Ex. 6 timer
» Time executables with: `time ./main`

12 Python

» Get help using `help(), help(int), help(object)`

List

```
x = [0, 1, 2, 3, 3] # list
x[2] == 2
x.insert(0, 5) # insert(ind, val) [5, 0, 1, 2, 3, 3]
x.pop(0) # [0, 1, 2, 3, 3]
x = [0, 1, 2, 'three'] # any types
x[-2] == 2 # negative index -> access from back
x += [4, 5, 6] # [0, 1, 2, 'three', 4, 5, 6]
x[1:4] # [start:end+1] [1, 2, 'three']
x[1:] # [start:end] [1, 2, 3, ,'three', 4, 5, 6]
x[0:-1] # [start:end-1] [0, 1, 2, 'three', 4, 5]
x[0:7:4] == x[::4] # [start;end+1:step] [0, 4]
x[-1:0:-2] # reverse sliciing [6, 4, 2]
x[::-2] # [6, 4, 2, 0]
```

Tuples (immutable)

```
x = (1, 2, 3)
x[1] = 3 # type error, not possible
```

Dictionary

```
x = dict(a=1, b=2, c='three')
x = {'a':1, 'b':2, 'c':'three'}
x['a'] == 1
x[1] = 4 # adding new entry, any type can be key
x.keys() # ['a', 'c', 1, 'b'] # order not preserved
x.values() # [1, 'three', 4, 2]
x.items() # [('a', 1), ('c', 'three'),
            (1, 4), ('b', 2)]
```

for loop

```
for <item> in <collection>: <statements>
for item in [0, 'a', 7, 1j]: print(item)
for i in "StRiNg": print(i)
b = [i+1 for i in range(3) if i!=2] # [1, 2]
```

Functions

```
def func(a, b=2, c="default"):
    ...
    return ...
func(4); func(4, 5); func(4, 5, "yo"); func(4, 5, 6)
func(b=4,c=5,a=6) # out-of-order call
#variadic args
def fun(a, b=2, *args, c, d=4, **kwargs): ...
fun(positional_args, keyword_args) # call fun
```

a positional argument, b pos. arg. with default, args variadic positional args, c keyword-only arg, d keyword-only with default, kwargs variadic keyword-only argument

Lambda

```
def F(a, b): return a-b
F = lambda a, b: a - b
```

Classes

» ctor: `__init__`; dtor: `__del__`; op+: `__add__`; op*: `__mul__`; op/: `__truediv__`; //: `__floordiv__`
» don't forget `self` as first argument!
» cf. slide 12.56 Inheritance, Decorators (@expr) etc.

NumPy / Matplotlib: see cheatsheets & Demos (Week 13) & Slides 13a

Efficient access instead of loop

```
import numpy as np
a = np.linspace(1, 10, 10, dtype=float)
b = np.random.random(10) * 10
b[:] += a[::-1] # b[i] += a[n-i-1]
```