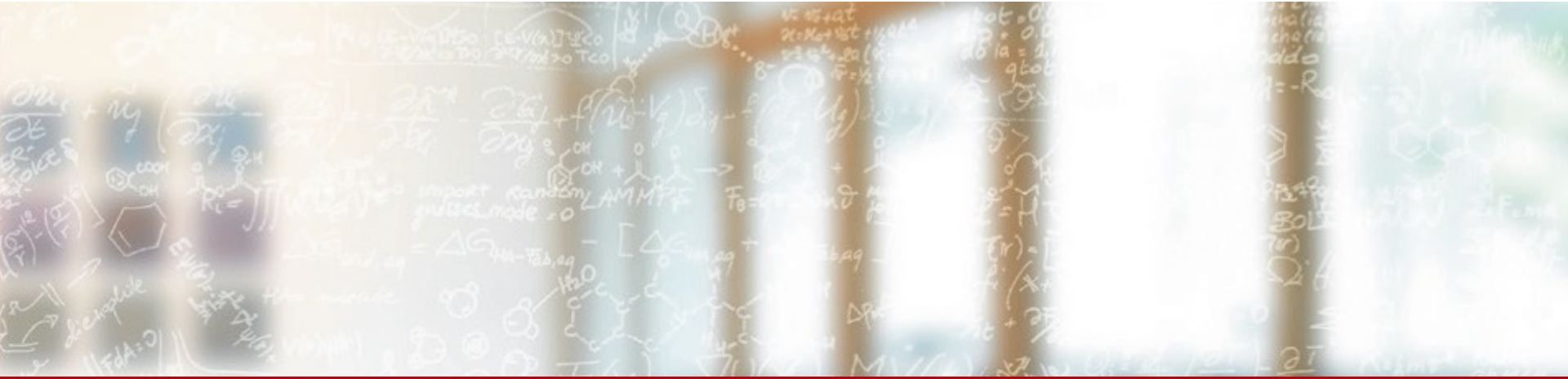




CSCS

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich



Advanced C++ for HPC

Advanced C++ for HPC

CSCS, Lugano, CH

Welcome to the Advanced C++ Course

- This year we are fully online!
- Approximate times
 - 9:00 – 10:30
 - 10:45 – 12:00
 - 13:00 – 14:30
 - 14:45 – 16:15
- During the breaks
 - <https://spatial.chat/s/CSCSch?sp=NetworkingSpace2021>

Practicals

- Examples and exercises can be found at
https://github.com/eth-cscs/examples_cpp
- Slides can be found at
See event page at cscs later during the course
- To compile
 - ``cd examples_cpp; mkdir build; cd build``
 - Run ``cmake ../Code``
 - Optionally `-DCMAKE_BUILD_TYPE=debug|release`
 - Then ``make``
 - ``make help``
 - ``make``

Feedback

- Do you use STL?
- Do you use C++ threads?
- Do you use templates?
- Do you use constexpr?
- Do you use patterns?

What is HPC?

- What is performance?

- Efficiency of resource utilization?
- Time to solution?
- Energy to solution?
- Algorithmic complexity?

- HPC modes

- Research codes
 - Prototyping oriented
 - Short runs
 - Results are architecture related information
 - Scientific results
 - Long runs
 - Results independent from hardware
 - Lifetime depend on publication of results
- Production applications and libraries
 - Long runs
 - Results independent from hardware
 - Lifetime spans multiple hardware generations

Programming language
and methodology
dictated by time to
deliver

Programming language
and methodology
dictated by long term
costs

Beware of the
transition

Programmers, CSs and SWEs

- Programmer
 - Knows how to program a computer
 - Knows at least one programming language well
- Computer Scientist
 - Understands algorithms, algorithm design, data structures
 - Understands computing machineries (at least in principle)
 - Can reason about complexity, performance, information theory...
- Software Engineer
 - Values the code as a self standing product to craft
 - Worries about maintenance and refactoring cost
 - Focuses on interfaces, reusability, composability
 - Enjoy clean code and receiving reviews for improving its quality

High Performance Code

```
for (int i = 0; i < n; ++i)
  for (int j = 0; j < m; ++j)
    for (int k = 0; k < l; ++k)
      c[i][j] += a[i][k] * b[k][j];
(a)
```

```
for (int i = 0; i < n; ++i)
  for (int k = 0; k < l; ++k)
    for (int j = 0; j < m; ++j)
      c[i][j] += a[i][k] * b[k][j];
(b)
```

- Which is faster?
 1. (a)
 2. (b)
 3. The same (the order would not matter)
 4. The same (the C++ compiler understands)

Bottom line: use BLAS!

C++ is not making writing HPC code easier!

HPC Focuses on Hardware

- C++ started providing system related information
 - **`std::thread::hardware_concurrency`**
 - Minimum offset between two objects to avoid false sharing
 - **`std::hardware_destructive_interference_size`**
 - Maximum size of contiguous memory to promote true sharing
 - **`std::hardware_constructive_interference_size`**
 - Number of concurrent threads supported
- Not a programming model yet

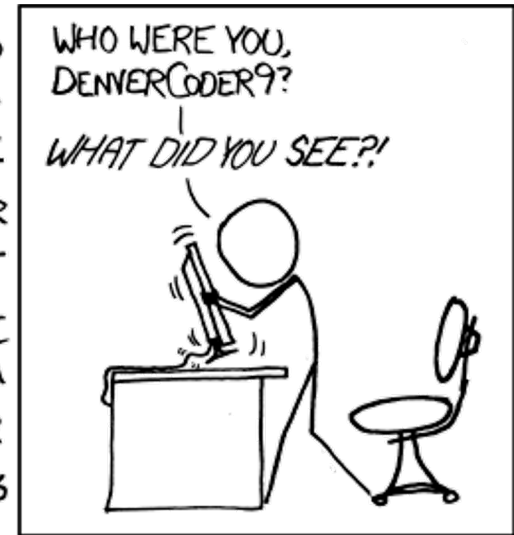
What is C++

- Programming language that allows
- Overhead-free abstractions
 - Or minimal overhead given the constraints
- Development of safe and robust code
 - Mostly by allowing good methodologies (such as RAI)
 - Constrained by performance requirements

Why C++?

- Supported by hardware
- Integrated in established IDEs
- Many available compilers
- Huge online community
- Scales with application complexity
 - Control investment by isolating components
 - Allows API design and implementation
 - Thanks to overhead free abstractions

NEVER HAVE I FELT SO
CLOSE TO ANOTHER SOUL
AND YET SO HELPLESSLY ALONE
AS WHEN I GOOGLE AN ERROR
AND THERE'S ONE RESULT
A THREAD BY SOMEONE
WITH THE SAME PROBLEM
AND NO ANSWER
LAST POSTED TO IN 2003

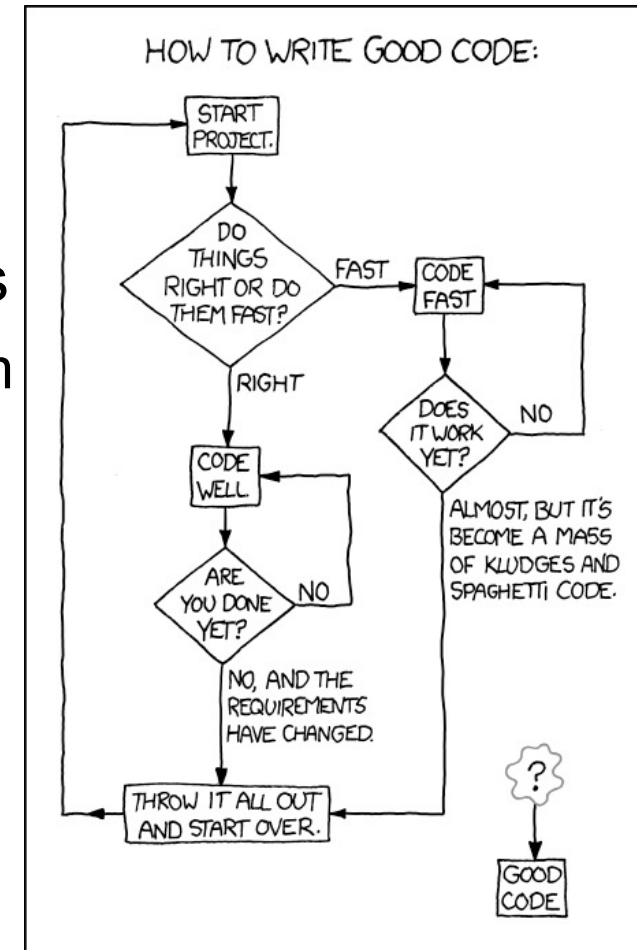


C++...

- Rise abstraction level
 - Leads to declarative style programming
- Library adaptation/abstraction
- **Separation of concerns**
- **Fast prototyping straight into production**
- **Incremental optimization / Extensibility**
- Downside: **typical HPC tools fails**
 - Mostly due to massive inlining

There should not be C++ without

- API design
- Unit testing
- Test Driven Development
- Systematic application of methodologies
 - Limit violations and always try to fix them
- Coding standards
- This course is in this context!



Unit Testing

- Every component, or sub-component, function, facility...

Should be tested!

- Examples:
 - A function to compute a value
 - A data-member that should satisfy an invariant
 - A value that should always be available at compile time
- Few things can not be unit-tested
 - `int main()`
 - Keep main at short
 - `static_assert`
- Use a unit-testing framework!
 - C++ does not offer one

```
int getRandomNumber()  
{  
    return 4; // chosen by fair dice roll.  
             // guaranteed to be random.  
}
```

Test-Driven Design/Development (TDD)

- **Before developing a feature write the code that uses it!**
- Lead to better APIs
 - Think as a user that's not you
- APIs are the most **durable** things you'll develop
 - For the good or for the bad
 - Believe it or not you are API designers
- I also do DDD: Desire-Driven Design
 - Fix interface if my wish is not realizable
- KISS: Keep It Simple St..id

A Good API Should

- **Be easy to use correctly**

- Intuitive and self explanatory
 - `list.size()` vs. `list.real_size()`
 - `list.length()` vs. `list.maximum_length()`
- Check for error conditions
- Signal the errors appropriately
 - `static_assert`, `asserts`, `exceptions`, `error codes`

- **Difficult to use mistakenly**

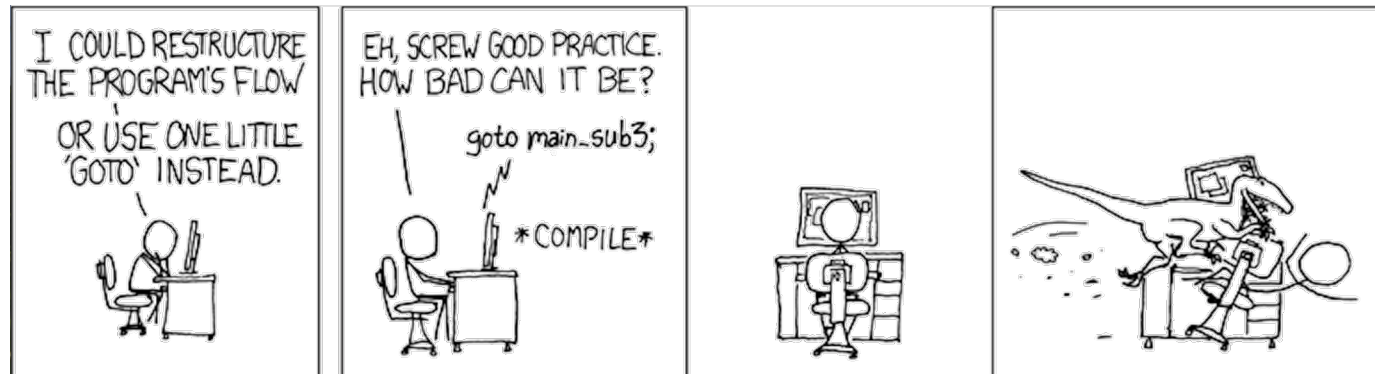
- Using protections to catch common misuses
- Be simple (see next)

- Documentation is useful if

- User read it
- User can remember some of it (API must be simple)

Methodologies I: Adhere to rules (examples that may apply)

- Always implement classes that provide RAI
 - A user of that class never needs a **new** statement
- Every function should be at most **n** lines long
- A class should do at most **n** things
- Write code that comment itself (comment the rest)
- Review code upon pull-requests
- Run automatic tests suites
- And more...



Hello world

```
#include <iostream>
```

Using at
global scope

```
using namespace std;
```

Useless
comment

```
/*  
 * main function  
 */
```

Useless
comment

```
int main() {  
    cout << "Hello world!" << endl; // Prints hello world  
    return 0;  
}
```

Superfluous
and not
portable

Use '\n'

Global
variable (ok
in main)

Methodologies II: Function Design (examples that may apply)

- Function names should be meaningful
- Number of arguments (< 4)
- Don't pass `const& int`
- **`set_time(int year, int month, int day)`**
 - `set_time(10,7,2012)`: what is the meaning?
- **`set_time(Year year, Month month, Day day)`**
 - `set_time(Day(10), Month(7), Year(2012))`
 - Don't provide conversions
- Call it **`set_date`** maybe?

Methodologies III: Class Design

- Implement “Concrete Types”
 - Behaves like an int
- Rule of 0
 - A class that does not need special constructors or destructors does not need to specify any
- Rule of 3
 - If your class needs a user defined copy, copy-assign or a destructor then it probably needs all three
- Rule of 5
 - If an object needs to be moved, then all 5 are needed: copy, copy-assign, move, move-assign, destructor

Automatic generation of special member functions

- Default constructor if no other constructor is explicitly declared
- Copy constructor if no move constructor and move assignment operator are explicitly declared
- If a destructor is declared generation of a copy constructor is deprecated
- Move constructor if no copy constructor, copy assignment operator, move assignment operator and destructor are explicitly declared
- Copy assignment operator if no move constructor and move assignment operator are explicitly declared
- Move assignment operator if no copy constructor, copy assignment operator, move constructor and destructor are explicitly declared
- Destructor

Methodologies IV: RAII

- Encapsulate each resource into a class, where
- Constructor acquires the resource
 - Also establishes all class invariants or throws
- Destructor releases the resource and never throws
- Always use the resource via an instance of a RAII-class
- RAII-class either
 - Automatic or temporary storage duration
 - Lifetime bounded by that of an automatic or temporary object
- Well defined by initialization order, stack-unwinding...
- Made effective by move semantics

Coding Conventions: Religion at test

- **Needed to make code readable**
 - Reduce time waste on small details
 - You'll now the kind of symbol by the syntax, example:
 - 'm_name' is a data member
 - 's_name' is a static member
 - 'Name' is a template argument
 - Common spacing across the project
- There are many coding conventions out there
- Find consensus in your team
 - Then cut it off
- Try not to be an extremist
 - The aim is to make code readable!

Design Patterns/Idioms

- C++ provide many patterns few are relevant for HPC
 - CRTP
 - Type Erasure
 - Proxy
 - Visitor

What We Cover... more or less

- Object Initialization
- Name resolution
- Templates
- Move semantics
- Smart Pointers
- Threads
- Tasking library
- Constexpr
- Lambdas/Functions
- STL
- Generic Programming/Concepts
- Several use cases

Thinking C++

- Some behaviors in C++ may seem abstruse
- But they –almost always– have a good reason
 - Typically for efficiency!
 - Compatibility with C
- We need a **mental model** for reasoning about code
- Most of this model comes from low level details
 - Function call mechanisms
 - Stack frames
 - Optimization techniques
 - String matching and substitution
 - Maybe even Godelization
- Sometimes we can live with **approximate models**