Research Computing with C++

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Contents

Chapter 1

C++ for Research

Course Overview

Part 1

- Correct C++ via unit testing
- Very brief C++ recap
- Reliable C++
- Reproducible science

Part 2

- HPC concepts
- Shared memory parallelism - OpenMP
- Distributed memory parallelism - MPI
- Accelerators (GPU/Thrust)
- Cloud Computing - Amazon EC2

Course Aims

- Teach how to do research with C++
- Optimise your research output
- A taster for a lot of technologies
- Not just C++ syntax, Google/Compiler could tell you that!

Pre-requisites

- You are already doing some C++
- You are familiar with your compiler
- You are happy with the concept of classes
- You know C++ up to templates?
- You are familiar with development eg. version control
  - Git: https://git-scm.com/

Course Notes

- Software Engineering: MPHYG001
- UCL Moodle: MPHYG002
- Online notes: MPHYG002

Course Assessment

- 3 hour exam
- 2 pieces coursework - 40 hours each
  - 1 due 3rd week March
  - 1 due last week April

Course Community

- UCL Research Programming Hub: http://research-programming.ucl.ac.uk
- Slack: https://ucl-programming-hub.slack.com

Todays Lesson

- Introduction, course overview, admin
- Using C++ in research
- Using Git
- Using CMake
- Using Catch unit testing framework

C++ In Research

Problems In Research

- Poor quality software

- Excuses
  - I'm not a software engineer
  - I don't have time
  - I'm unsure of my code

C++ Disadvantages

Some people say:

- Compiled language
  - (compiler versions, libraries, platform specific etc)
- Perceived as difficult, error prone, wordy, unfriendly syntax
- Result: It's more trouble than its worth?

C++ Advantages

- Fast, code compiled to machine code
- Nice integration with CUDA, OpenACC, OpenCL, OpenMP, OpenMPI
- Stable, evolving standard, powerful notation, improving
- Lots of libraries, Boost, Qt, VTK, ITK etc.
- Result: Good reasons to use it, or you may *have* to use it

Research Programming

- Software is already expensive
  - Famous Book: Mythical Man Month
  - Famous People: Edsger W. Dijkstra
- Research programming is different
  - What is the end product?

Development Methodology?

- Will software engineering methods help?
  - Waterfall
  - Agile
- At the 'concept discovery' stage, probably too early to talk about product development

Approach

- What am I trying to achieve?
- How do I maximise my output?
- What is the best pathway to success?
- How do I de-risk my research?

1. Types of Code

- What are you trying to achieve?
- Divide code:
  - Your algorithm: NiftyReg
  - Testing code
  - Data analysis
  - User Interface
  - Glue code
  - Deployment code
  - Scientific paper production

Examples: NiftyReg 300 citations in 5 years!

2. Maximise Your Value

- Developer time is expensive
- Your brain is your asset
- Write as little code as possible
- Focus tightly on your hypothesis
- Write the minimum code that produces a paper

Don't fall into the trap "Hey, I'll write a framework for that"

3. Ask Advice

- Before contemplating a new piece of software
  - Ask advice - Slack Channel
  - Review libraries and use them.
  - Check libraries are suitable, and sustainable.
  - Read Libraries section from Software Engineering course
  - Ask about best practices

Example - NiftyCal

- We should: Practice What We Preach
- Small, algorithms
- Unit tested
- Version controlled
- Small number of libraries
- Increased research output

Debunking The Excuses

- I'm not a software engineer
  - Learn effective, minimal tools
- I don't have time
  - Unit testing to save time
  - Choose your battles/languages wisely
- I'm unsure of my code
  - Share, collaborate

What Isn't This Course?

We are NOT suggesting that:

- C++ is the solution to all problems.
- You should write all parts of your code in C++.

What Is This Course?

We aim to:

- Improve your C++ (and associated technologies).
- Do High Performance Computing (HPC).

So that:

- Apply it to research in a pragmatic fashion.
- You use the right tool for the job.

Git

Git Introduction

- This is a practical course
- We will use git for version control
- Submit git repository for coursework
- Here we provide a very minimal introduction

Git Resources

- Complete beginner - Try Git
- Git book by Scott Chacon
- Git section of MPHYG001
- MPHYG001 repo

Git Walk Through

(demo on command line)

- git init
- git add
- git commit
- git status
- git log
- git push
- git pull
- git clone
- forking

Homework

- Register Github
- Create new empty repository - CPPCW1
- Ensure it is a private repository - free
- Find project of interest - try cloning it
- Find project of interest - try forking it

CMake

CMake Introduction

- This is a practical course
- We will use CMake as a build tool
- CMake produces
  - Windows: Visual Studio project files
  - Linux: Make files
  - Mac: XCode projects, Make files
- This course will provide CMake code and boiler plate code

CMake Usage Linux/Mac

Demo an "out-of-source" build

```
cd ~/build
git clone https://github.com/MattClarkson/CMakeHelloWorld
mkdir CMakeHelloWorld-build
cd CMakeHelloWorld-build
ccmake ../CMakeHelloWorld
make
```

CMake Usage Windows

Demo an "out-of-source" build

- git clone https://github.com/MattClarkson/CMakeHelloWorld
- Run cmake-gui.exe
- Select source folder (CMakeHelloWorld downloaded above)
- Specify new build folder (CMakeHelloWorld-build next to, but not inside CMakeHelloWorld)
- Hit *configure*
- When asked, specify compiler
- Set flags and repeatedly *configure*
- When *generate* option is present, hit *generate*
- Compile, normally using Visual Studio

Unit Testing

What is Unit Testing?

At a high level

- Way of testing code.
- Unit
  - Smallest 'atomic' chunk of code
  - i.e. Function, could be a Class
- See also:
  - Integration/System Testing
  - Regression Testing
  - User Acceptance Testing

Benefits of Unit Testing?

- Certainty of correctness
- (Scientific Rigour)
- Influences and improves design
- Confidence to refactor, improve

Drawbacks for Unit Testing?

- Don't know how
  - This course will help
- Takes too much time
  - Really?
  - IT SAVES TIME in the long run

Unit Testing Frameworks

Generally, all very similar

- JUnit (Java), NUnit (.net?), CppUnit, phpUnit,
- Basically
  - Macros (C++), methods (Java) to test conditions
  - Macros (C++), reflection (Java) to run/discover tests

- Ways of looking at results.
    * Java/Eclipse: Integrated with IDE
    * Log file or standard output

Unit Testing Example

How To Start

We discuss

- Basic Example
- Some tips

Then its down to the developer/artist.

C++ Frameworks

To Consider:

- Catch
- GoogleTest
- QTestLib
- BoostTest
- CppTest
- CppUnit

Worked Example

- Borrowed from
    - Catch Tutorial
    - and Googletest Primer
- We use Catch, so notes are compilable
- But the concepts are the same

Code

To keep it simple for now we do this in one file:

```
#define CATCH_CONFIG_MAIN  // This tells Catch to provide a main() - only do this in one cpp
#include "../catch/catch.hpp"

unsigned int Factorial( unsigned int number ) {
    return number <= 1 ? number : Factorial(number-1)*number;
}

TEST_CASE( "Factorials are computed", "[factorial]" ) {
    REQUIRE( Factorial(1) == 1 );
    REQUIRE( Factorial(2) == 2 );
    REQUIRE( Factorial(3) == 6 );
    REQUIRE( Factorial(10) == 3628800 );
}
```

Produces this output when run:

```
===============================================================================
All tests passed (4 assertions in 1 test case)
```

Principles

So, typically we have

- Some `#include` to get test framework
- Our code that we want to test
- Then make some assertions

Catch / GoogleTest

For example, in Catch:

```
// TEST_CASE(<unique test name>, <test case name>)
TEST_CASE( "Factorials are computed", "[factorial]" ) {
    REQUIRE( Factorial(2) == 2 );
    REQUIRE( Factorial(3) == 6 );
}
```

In GoogleTest:

```
// TEST(<test case name>, <unique test name>)
TEST(FactorialTest, HandlesPositiveInput) {
```

```
    EXPECT_EQ(2, Factorial(2));
    EXPECT_EQ(6, Factorial(3));
  }
```

all done via C++ macros.

Tests That Fail

What about Factorial of zero? Adding

```
REQUIRE( Factorial(0) == 1 );
```

Produces something like:

```
factorial2.cc:9: FAILED:
REQUIRE( Factorial(0) == 1 )
with expansion:
0 == 1
```

Fix the Failing Test

Leading to:

```
#define CATCH_CONFIG_MAIN  // This tells Catch to provide a main() - only do this in one cpp
#include "../catch/catch.hpp"

unsigned int Factorial( unsigned int number ) {
    //return number <= 1 ? number : Factorial(number-1)*number;
    return number > 1 ? Factorial(number-1)*number : 1;
}

TEST_CASE( "Factorials are computed", "[factorial]" ) {
    REQUIRE( Factorial(0) == 1 );
    REQUIRE( Factorial(1) == 1 );
    REQUIRE( Factorial(2) == 2 );
    REQUIRE( Factorial(3) == 6 );
    REQUIRE( Factorial(10) == 3628800 );
}
```

which passes:

```
===============================================================================
All tests passed (5 assertions in 1 test case)
```

Test Macros

Each framework has a variety of macros to test for failure. [Check][Check] has:

```
REQUIRE(expression); // stop if fail
CHECK(expression);   // doesn't stop if fails
```

if an exception is throw, its caught, reported and counts as a failure.

Examples:

```
CHECK( str == "string value" );
CHECK( thisReturnsTrue() );
REQUIRE( i == 42 );
```

Others:

```
REQUIRE_FALSE( expression )
CHECK_FALSE( expression )
REQUIRE_THROWS( expression ) # Must throw an exception
CHECK_THROWS( expression ) # Must throw an exception, and continue testing
REQUIRE_THROWS_AS( expression, exception type )
CHECK_THROWS_AS( expression, exception type )
REQUIRE_NOTHROW( expression )
CHECK_NOTHROW( expression )
```

Testing for Failure

To re-iterate:

- You should test failure cases
  - Force a failure
  - Check that exception is thrown
  - If exception is thrown, test passes
  - (Some people get confused, expecting test to fail)
- Examples
  - Saving to invalid file name
  - Negative numbers passed into double arguments
  - Invalid Physical quantities (e.g. -300 Kelvin)

Setup/Tear Down

- Some tests require objects to exist in memory
- These should be set up
  - for each test
  - for a group of tests
- Frameworks do differ in this regards

Setup/Tear Down in Catch

Referring to the Catch Tutorial:

```
TEST_CASE( "vectors can be sized and resized", "[vector]" ) {

    std::vector<int> v( 5 );

    REQUIRE( v.size() == 5 );
    REQUIRE( v.capacity() >= 5 );

    SECTION( "resizing bigger changes size and capacity" ) {
        v.resize( 10 );

        REQUIRE( v.size() == 10 );
        REQUIRE( v.capacity() >= 10 );
    }
    SECTION( "resizing smaller changes size but not capacity" ) {
        v.resize( 0 );

        REQUIRE( v.size() == 0 );
        REQUIRE( v.capacity() >= 5 );
    }
    SECTION( "reserving bigger changes capacity but not size" ) {
        v.reserve( 10 );

        REQUIRE( v.size() == 5 );
        REQUIRE( v.capacity() >= 10 );
    }
    SECTION( "reserving smaller does not change size or capacity" ) {
        v.reserve( 0 );

        REQUIRE( v.size() == 5 );
        REQUIRE( v.capacity() >= 5 );
    }
}
```

So, Setup/Tear down is done before/after each section.

Unit Testing Tips

C++ design

- Stuff from above applies to Classes / Functions
- Think about arguments:
    - Code should be hard to use incorrectly.
    - Use `const`, `unsigned` etc.
    - Testing forces you to sort these out.

Test Driven Development (TDD)

- Methodology
    1. Write a test
    2. Run test, should fail
    3. Implement/Debug functionality
    4. Run test
        1. if succeed goto 5
        2. else goto 3
    5. Refactor to tidy up

TDD in practice

- Aim to get good coverage
- Some people quote 70% or more
- What are the downsides?
- Don't write 'brittle' tests

Behaviour Driven Development (BDD)

- Behaviour Driven Development (BDD)
    - Refers to a whole area of software engineering
    - With associated tools and practices
    - Think about end-user perspective
    - Think about the desired behaviour not the implementation
    - See Jani Hartikainen article.

TDD Vs BDD

- TDD
  - Test/Design based on methods available
  - Often ties in implementation details
- BDD
  - Test/Design based on behaviour

  - Code to interfaces (later in course)
- Subtly different
- Aim for BDD

Anti-Pattern 1: Setters/Getters

Testing every Setter/Getter.

Consider:

```
class Atom {

  public:
    void SetAtomicNumber(const int& number) { m_AtomicNumber = number; }
    int GetAtomicNumber() const { return m_AtomicNumber; }
    void SetName(const std::string& name) { m_Name = name; }
    std::string GetName() const { return m_Name; }
  private:
    int m_AtomicNumber;
    std::string m_Name;
};
```

and tests like:

```
TEST_CASE( "Testing Setters/Getters", "[Atom]" ) {

    Atom a;

    a.SetAtomicNumber(1);
    REQUIRE( a.GetAtomicNumber() == 1);
    a.SetName("Hydrogen");
    REQUIRE( a.GetName() == "Hydrogen");
```

- It feels tedious

- But you want good coverage
- This often puts people off testing
- It also produces "brittle", where 1 change breaks many things

Anti-Pattern 1: Suggestion.

- Focus on behaviour.
    - What would end-user expect to be doing?
    - How would end-user be using this class?
    - Write tests that follow the use-case
    - Gives a more logical grouping
    - One test can cover > 1 function
    - i.e. move away from slavishly testing each function
- Minimise interface.
    - Provide the bare number of methods
    - Don't provide setters if you don't want them
    - Don't provide getters unless the user needs something
    - Less to test. Use documentation to describe why.

Anti-Pattern 2: Constructing Dependent Classes

- Sometimes, by necessity we test groups of classes
- Or one class genuinely Has-A contained class
- But the contained class is expensive, or could be changed in future

Anti-Pattern 2: Suggestion

- Read up on [Dependency Injection][DependencyInjection]
- Enables you to create and inject dummy test classes
- So, testing again used to break down design, and increase flexibility

Summary BDD Vs TDD

Aim to write:

- Most concise description of requirements as unit tests
- Smallest amount of code to pass tests
- ... i.e. based on behaviour

Any Questions?

End of Lecture?

- Example git repo, CMake, Catch template project:
  - https://github.com/MattClarkson/CMakeCatchTemplate

Chapter 2

Better C++

Better C++

Last Weeks Lesson

- Getting started
- Git
- CMake
- Unit Testing

Todays Lesson

- Beginners C++ not sufficient
- Look at
  - C++ recap
  - Templates - generic programming
  - Exceptions - error handling
  - Construction

Object Oriented Review

C-style Programming

- Procedural programming
- Pass data to functions

Function-style Example

```
double compute_similarity(double *imag1, double* image2, double *params)
{
  // stuff
}

double calculate_derivative(double* params)
{
  // stuff
}

double convert_to_decimal(double numerator, double denominator)
{
  // stuff
}
```

Disadvantages

- Can get out of hand as program size increases
- Can't easily describe relationships between bits of data
- Relies on method documentation, function and variable names
- Can't easily control/(enforce control of) access to data

C Struct

- So, in C, the struct was invented
- Basically a class without methods
- This at least provides a logical grouping

Struct Example

```
struct Fraction {
  int numerator;
  int denominator;
};

double convertToDecimal(const Fraction& f)
{
  return f.numerator/static_cast<double>(f.denominator);
}
```

C++ Class

- C++ provides the class to enhance the language with user defined types
- Once defined, use types as if native to the language

Abstraction

- C++ class mechanism enables you to define a type
  - independent of its data
  - independent of its implementation
  - class defines concept or blueprint
  - instantiation creates object

Abstraction - Grady Booch

"An abstraction denotes the essential characteristics of an object that distinguish it from all other kinds of objects and thus provide crisply defined conceptual boundaries, relative to the perspective of the viewer."

Class Example

```
class Atom {
public:
  Atom(){};
  ~Atom(){};
  int GetAtomicNumber();
  double GetAtomicWeight();
};

int main(int argc, char** argv)
{
  Atom a;
}
```

Encapsulation

- Encapsulation is:
  - Bundling together methods and data
  - Restricting access, defining public interface
- Describes how you correctly use something

Public/Private/Protected

- For class methods/variables:
  - `private`: only available in this class
  - `protected`: available in this class and derived classes
  - `public`: available to anyone with access to the object
- (public, protected, private inheritance comes later)

Class Example

```
// Defining a User Defined Type.
class Fraction {

public: // access control

  // How to create
  Fraction();
  Fraction(const int& num, const int& denom);

  // How to destroy
  ~Fraction();

  // How to access
  int numerator() const;
  int denominator() const;

  // What you can do
  const Fraction operator+(const Fraction& another);

private: // access control

  // The data
  int m_Numerator;
  int m_Denominator;
};
```

Inheritance

- Used for:
  - Defining new types based on a common type
- Careful:
  - Beware - "Reduce code duplication, less maintenance"

    - Types in a hierarchy MUST be related
    - Don't over-use inheritance
    - We will cover other ways of object re-use

Class Example

```
class Shape {
  public:
    Shape();
    void setVisible(const bool& isVisible) { m_IsVisible = isVisible; }
    virtual void rotate(const double& degrees) = 0;
    virtual void scale(const double& factor) = 0;
    // + other methods
  private:
    bool m_IsVisible;
    unsigned char m_Colour[3]; // RGB
    double m_CentreOfMass[2];
};

class Rectangle : public Shape {
  public:
    Rectangle();
    virtual void rotate(const double& degrees);
    virtual void scale(const double& factor);
    // + other methods
  private:
    double m_Corner1[2];
    double m_Corner2[2];
};

class Circle : public Shape {
  public:
    Circle();
    virtual void rotate(const double& degrees);
    virtual void scale(const double& factor);
    // + other methods
  private:
    float radius;
};
```

Polymorphism

- Several types:
    - (normally) "subtype": via inheritance

  - “parametric”: via templates
  - “ad hoc”: via function overloading

- Common interface to entities of different types
- Same method, different behaviour

Class Example

```
#include "shape.h"
int main(int argc, char** argv)
{
  Circle c1;
  Rectangle r1;
  Shape *s1 = &c1;
  Shape *s2 = &r1;

  // Calls method in Shape (as not virtual)
  bool isVisible = true;
  s1->setVisible(isVisible);
  s2->setVisible(isVisible);

  // Calls method in derived (as declared virtual)
  s1->rotate(10);
  s2->rotate(10);
}
```

Essential Reading

General Advice

- Do a version control course such as Software Carpentry, or MPHYG001.
- Contribute to online open-source project
- For your repository - pick a coding style, and stick to it

Daily Reading

- Every C++ developer should keep repeatedly reading at least:
  - Effective C++, Meyers
  - More Effective C++, Meyers
  - Effective STL, Meyers

Additional Reading

- Recommended
  - Accelerated C++, Koenig, Moo.
  - Design Patterns (1994), Gamma, Help, Johnson and Vlassides
  - Modern C++ Design, Andrei Alexandrescu

C++ tips

Numbers in brackets refer to Scott Meyers "Effective C++" book.

- Top C++ tips such as:
  - Declare data members private (22)
  - Use `const` whenever possible (3)
  - Make interfaces easy to use correctly and hard to use incorrectly (18)
  - Avoid returning "handles" to object internals (28)
  - Initialise objects properly. Throw exceptions from constructors. Fail early. (4)

OO tips

- More general OO tips such as:
  - Never throw exceptions from destructors
  - Prefer non-member non-friend functions to member functions (better encapsulation) (23)
  - Make sure public inheritance really models "is-a" (32)
  - Learn alternatives to polymorphism (Template Method, Strategy) (35)
  - Model "has-a" through composition (38)

Using Templates

What Are Templates?

- C++ templates allow functions/classes to operate on generic types.
- See: Generic Programming.
- Write code, where 'type' is provided later
- Types instantiated at compile time, as they are needed
- (Remember, C++ is strongly typed)

You May Already Use Them!

You probably use them already. Example type (class):

```
std::vector<int> myVectorInts;
```

Example algorithm: C++ sort

```
std::sort(myVectorInts.begin(), myVectorInts.end());
```

Aim: Write functions, classes, in terms of future/other/generic types, type provided as parameter.

Why Are Templates Useful?

- Generic programming:
  - not pre-processor macros
  - so maintain type safety
  - separate algorithm from implementation
  - extensible, optimisable via Template Meta-Programming (TMP)

Book

- You should read "Modern C++ Design"
- 2001, but still excellent text on templates, meta-programming, policy based design etc.
- This section of course, gives basic introduction for research programmers

Are Templates Difficult?

- Some say: notation is ugly
  - Does take getting used to
  - Use `typedef` to simplify
- Some say: verbose, confusing error messages
  - Nothing intrinsically difficult
  - Take small steps, compile regularly
  - Learn to think like a compiler
- Code infiltration
  - Use sparingly
  - Hide usage behind clean interface

Why Templates in Research?

- Generalise 2D, 3D, n-dimensions, (e.g. ITK)
- Test numerical code with simple types, apply to complex/other types
- Several useful libraries for research

Why Teach Templates?

- Standard Template Library uses them
- More common in research code, than business code
- In research, more likely to 'code for the unknown'
- Boost, Qt, EIGEN uses them

Function Templates

Function Templates Example

- Credit to www.cplusplus.com

```
// function template
#include <iostream>
using namespace std;

template <class T> // class/typename
T sum (T a, T b)
{
  T result;
  result = a + b;
  return result;
}

int main () {
  int i=5, j=6;
  double f=2.0, g=0.5;
  cout << sum<int>(i,j) << '\n';
  cout << sum<double>(f,g) << '\n';
  return 0;
}
```

- And produces this output when run

```
11
2.5
```

Why Use Function Templates?

- Instead of function overloading
  - Reduce your code duplication
  - Reduce your maintenance
  - Reduce your effort
  - Also see this Additional tutorial.

Language Definition 1

- From the language reference

```
template < parameter-list > function-declaration
```

- so

```
template < class T >  // note 'class'
void MyFunction(T a, T b)
{
  // do something
}
```

- or

```
template < typename T1, typename T2 >  // note 'typename'
T1 MyFunctionTwoArgs(T1 a, T2 b)
{
  // do something
}
```

Language Definition 2

- Also
  - Can use `class` or `typename`.
  - I prefer `typename`.
  - Template parameter can apply to references, pointers, return types, arrays etc.

Default Argument Resolution

- Given:

```
double GetAverage<typename T>(const std::vector<T>& someNumbers);
```

- then:

```
std::vector<double> myNumbers;
double result = GetAverage(myNumbers);
```

- will call:

```
double GetAverage<double>(const std::vector<double>& someNumbers);
```

- So, if function parameters can inform the compiler uniquely as to which function to instantiate, its automatically compiled.

Explicit Argument Resolution - 1

- However, given:

```
double GetAverage<typename T>(const T& a, const T& b);
```

- and:

```
int a, b;
int result = GetAverage(a, b);
```

- But you don't want the int version called (due to integer division perhaps), you can:

```
double result = GetAverage<double>(a, b);
```

Explicit Argument Resolution - 2

- equivalent to

```
GetAverage<double>(static_cast<double>(a), static_cast<double>(b));
```

- i.e. name the template function parameter explicitly.
- Cases for Explicit Template Argument Specification
  - Force compilation of a specific version (eg. int as above)
  - Also if method parameters do not allow compiler to deduce anything eg. `PrintSize()` method.

Beware of Code Bloat

- Given:

```
double GetMax<typename T1, typename T2>(const &T1, const &T2);
```

- and:

```
double r1 = GetMax(1,2);
double r2 = GetMax(1,2.0);
double r3 = GetMax(1.0,2.0);
```

- The compiler will generate 3 different max functions.
- Be Careful
  - Executables/libraries get larger
  - Compilation time will increase
  - Error messages get more verbose

Two Stage Compilation

- Basic syntax checking (eg. brackets, semi-colon, etc), when `#include`'d
- But only compiled when instantiated (eg. check existence of + operator).

Instantiation

- Object Code is only really generated if code is used
- Template functions can be
  - .h file only
  - .h file that includes separate .cxx/.txx/.hxx file (e.g. ITK)
  - .h file and separate .cxx/.txx file (sometimes by convention a .hpp file)
- In general
  - Most libraries/people prefer header only implementations

Explicit Instantiation - 1

- Language Reference here
- Microsoft Example

- Given (library) header:

```
#ifndef explicitInstantiation_h
#define explicitInstantiation_h
template<typename T> void f(T s);
#endif
```

- Given (library) implementation:

```
#include <iostream>
#include <typeinfo>
#include "explicitInstantiation.h"
template<typename T>
void f(T s)
{
    std::cout << typeid(T).name() << " " << s << '\n';
}
template void f<double>(double); // instantiates f<double>(double)
template void f<>(char); // instantiates f<char>(char), template argument deduced
template void f(int); // instantiates f<int>(int), template argument deduced
```

Explicit Instantiation - 2

- Given client code:

```
#include <iostream>
#include "explicitInstantiation.h"

int main(int argc, char** argv)
{
  std::cout << "Matt, double 1.0=" << std::endl;
  f(1.0);
  std::cout << "Matt, char a=" << std::endl;
  f('a');
  std::cout << "Matt, int 2=" << std::endl;
  f(2);
//  std::cout << "Matt, float 3.0=" << std::endl;
//  f<float>(static_cast<float>(3.0));  // compile error
}
```

- We get:

```
Matt, double 1.0=
```

```
d 1
Matt, char a=
c a
Matt, int 2=
i 2
```

Explicit Instantiation - 3

- Explicit Instantiation:
  - Forces instantiation of the function
  - Must appear after the definition
  - Must appear only once for given argument list
  - Stops implicit instantiation
- So, mainly used by compiled library providers
- Clients then `#include` header and link to library

```
Linking CXX executable explicitInstantiationMain.x
Undefined symbols for architecture x86_64:
  "void f<float>(float)", referenced from:
```

Implicit Instantiation - 1

- Instantiated as they are used
- Normally via `#include` header files.
- Given (library) header, that containts implementation:

```
#ifndef explicitInstantiation_h
#define explicitInstantiation_h
#include <iostream>
#include <typeinfo>
template<typename T>
void f(T s)
{
    std::cout << typeid(T).name() << " " << s << '\n';
}
#endif
```

Implicit Instantiation - 2

- Given client code:

```
#include <iostream>
#include "implicitInstantiation.h"

int main(int argc, char** argv)
{
  std::cout << "Matt, double 1.0=" << std::endl;
  f(1.0);
  std::cout << "Matt, char a=" << std::endl;
  f('a');
  std::cout << "Matt, int 2=" << std::endl;
  f(2);
  std::cout << "Matt, float 3.0=" << std::endl;
  f<float>(static_cast<float>(3.0));  // no compile error
}
```

- We get:

```
Matt, double 1.0=
d 1
Matt, char a=
c a
Matt, int 2=
i 2
Matt, float 3.0=
f 3
```

Class Templates

Class Templates Example - 1

- If you understand template functions, then template classes are easy!
- Refering to this tutorial, an example:

Header:

```
template <typename T>
class MyPair {
    T m_Values [2];
  public:
    MyPair(const T& first, const T& second);
    T getMax() const;
};
#include "pairClassExample.cc"
```

Class Templates Example - 2

Implementation:

```
template <typename T>
MyPair<T>::MyPair(const T& first, const T& second)
{
  m_Values[0] = first;
  m_Values[1] = second;
}

template <typename T>
T
MyPair<T>::getMax() const
{
  if (m_Values[0] > m_Values[1])
    return m_Values[0];
  else
    return m_Values[1];
}
```

Class Templates Example - 3

Usage:

```
#include "pairClassExample.h"
#include <iostream>

int main(int argc, char** argv)
{
  MyPair<int> a(1,2);
  std::cout << "Max is:" << a.getMax() << std::endl;
}
```

Quick Comments

- Implementation, 3 uses of parameter T
- Same Implicit/Explicit instantiation rules
- Note implicit requirements, eg. operator >
  - Remember the 2 stage compilation
  - Remember code not instantiated until its used
  - Take Unit Testing Seriously!

Template Specialisation

- If template defined for type T
- Full specialisation - special case for a specific type eg. char
- Partial specialisation - special case for a type that still templates, e.g. T*

```
template <typename T> class MyVector {
template <> class MyVector<char> {  // full specialisation
template <typename T> MyVector<T*> { // partial specialisation
```

Nested Types

In libraries such as ITK, we see:

```
template< typename T, unsigned int NVectorDimension = 3 >
class Vector:public FixedArray< T, NVectorDimension >
{
  public:
    // various stuff
    typedef T  ValueType;
    // various stuff
    T someMemberVariable;
```

- typedef is just an alias
- using nested typedef, must be qualified by class name
- can also refer to a real variable

Error Handling

Exceptions

- Exceptions are the C++ or Object Oriented way of Error Handling
- Read this example

Exception Handling Example

```
#include <stdexcept>
#include <iostream>
bool someFunction() { return false; }

int main()
```

```cpp
{
  try
  {
    bool isOK = false;
    isOK = someFunction();
    if (!isOK)
    {
      throw std::runtime_error("Something is wrong");
    }
  }
  catch (std::exception& e)
  {
    std::cerr << "Caught Exception:" << e.what() << std::endl;
  }
}
```

What's the Point?

- Have separated error handling logic from application logic
- First, lets look at C-style return codes

Error Handling C-Style

```cpp
int foo(int a, int b)
{
  // stuff

  if(some error condition)
  {
    return 1;
  } else if (another error condition) {
    return 2;
  } else {
    return 0;
  }
}

void caller(int a, int b)
{
 int result = foo(a, b);
 if (result == 1) // do something
 else if (result == 2) // do something difference
 else
```

```
  {
    // All ok, continue as you wish
  }
}
```

Outcome

- Can be perfectly usable
- Depends on depth of function call stack
- Depends on complexity of program
- If deep/large, then can become unweildy

Error Handling C++ Style

```cpp
#include <stdexcept>
#include <iostream>

int ReadNumberFromFile(const std::string& fileName)
{
  if (fileName.length() == 0)
  {
    throw std::runtime_error("Empty fileName provided");
  }

  // Check for file existence etc. throw io errors.

  // do stuff
  return 2; // returning dummy number to force error
}


void ValidateNumber(int number)
{
  if (number < 3)
  {
    throw std::logic_error("Number is < 3");
  }
  if (number > 10)
  {
    throw std::logic_error("Number is > 10");
  }
}
```

```cpp
int main(int argc, char** argv)
{
  try
  {
    if (argc < 2)
    {
      std::cerr << "Usage: " << argv[0] << " fileName" << std::endl;
      return EXIT_FAILURE;
    }

    int myNumber = ReadNumberFromFile(argv[1]);
    ValidateNumber(myNumber);

    // Compute stuff.

    return EXIT_SUCCESS;

  }
  catch (std::exception& e)
  {
    std::cerr << "Caught Exception:" << e.what() << std::endl;
  }
}
```

Outcome

- Code that throws does not worry about the catcher
- Exceptions are classes, can carry data
- Exceptions can form class hierarchy

Consequences

- More suited to larger libraries of re-usable functions
- Many different catchers, all implementing different error handling
- Lends itself to layered software (draw diagram)
- Generally scales better, more flexible

Practical Tips For Exception Handling

- Decide on error handling strategy at start
- Use it consistently
- Create your own base class exception

- Derive all your exceptions from that base class
- Stick to a few obvious classes, not one class for every single error

More Practical Tips For Exception Handling

- Look at C++ standard classes and tutorial
- An exception macro may be useful, e.g. mitk::Exception and mithThrow()
- Beware side-effects
  - Perform validation before updating any member variables

Inheritance

Don't overuse Inheritance

- Inheritance is not just for saving duplication
- It MUST represent derived/related types
- Derived class must truely represent 'is-a' relationship
- eg 'Square' is-a 'Shape'
- Deep inheritance hierarchies are almost always wrong
- If something 'doesn't quite fit' check your inheritance

Surely Its Simple?

- Common example: Square/Rectangle problem, here

```
#include <iostream>

class Rectangle {
public:
  Rectangle() : m_Width(0), m_Height(0) {};
  virtual ~Rectangle(){};
  int GetArea() const { return m_Width*m_Height; }
  virtual void SetWidth(int w) { m_Width=w; }
  virtual void SetHeight(int h) { m_Height=h; }
protected:
  int m_Width;
  int m_Height;
};

class Square : public Rectangle {
public:
```

```
  Square(){};
  ~Square(){};
  virtual void SetWidth(int w) { m_Width=w; m_Height=w; }
  virtual void SetHeight(int h) { m_Width=h; m_Height=h; }
};

int main()
{
  Rectangle *r = new Square();
  r->SetWidth(5);
  r->SetHeight(6);
  std::cout << "Area = " << r->GetArea() << std::endl;
}
```

Liskov Substitution Principal

- Wikipedia
- "if S is a subtype of T, then objects of type T may be replaced with objects of type S without altering any of the desirable properties of that program"
- Can something truely be substituted?
- If someone else filled a vector of type T, would I care what type I have?
- Look for:
  - Preconditions cannot be strengthened
  - Postconditions cannot be weakened
  - Invariants preserved

What to Look For

- If you have:
  - Methods you don't want to implement in derived class
  - Methods that don't make sense in derived class
  - Methods that are unneeded in derived class
  - If you have a list of something, and someone else swapping a derived type would cause problems
- Then you have probably got your inheritance wrong

Composition Vs Inheritance

- Lots of Info online eg. wikipedia
- In basic OO Principals
  - 'Has-a' means 'pointer or reference to'

  - eg.`Car` has-a `Engine`
- But there is also:
  - Composition: Strong 'has-a'. Component parts are owned by thing pointing to them.
  - Aggregation: Weak 'has-a'. Component part has its own lifecycle.
  - Association: General term, referring to either composition or aggregation, just a 'pointer-to'

Examples

- House 'has-a' set of Rooms. Destroying House, you destroy all Room objects. No point having a House on its own.
- Department 'has-a' Professor. If a department is shutdown (deleted), Professor should not be deleted. Needs assigning to another department.

But Why?

- Good article: Choosing Composition or Inheritance
- Inheritance has much tighter definition than you realise
- Composition is more flexible

Dependency Injection

Construction

- What could be wrong with this:

```
#include <memory>

class Bar {
};

class Foo {
public:
  Foo()
  {
    m_Bar = new Bar();
  }

private:
  Bar* m_Bar;
```

```
};

int main()
{
  Foo a;
}
```

Unwanted Dependencies

- If constructor instantiates class directly:
  - Hard-coded class name
  - Duplication of initialisation code

Dependency Injection

- Read Martin Fowler's Inversion of Control Containers and the Dependency Injection Pattern
- Type 2 - Constructor Injection
- Type 3 - Setter Injection

Constructor Injection Example

```
#include <memory>

class Bar {
};

class Foo {
public:
  Foo(Bar* b)
  : m_Bar(b)
  {
  }

private:
  Bar* m_Bar;
};

int main()
{
  Bar b;
```

```
  Foo a(&b);
}
```

Setter Injection Example

```
#include <memory>

class Bar {
};

class Foo {
public:
  Foo()
  {
  }
  void SetBar(Bar *b) { m_Bar = b; }

private:
  Bar* m_Bar;
};

int main()
{
  Bar b;
  Foo a();
  a.SetBar(&b);
}
```

Question: Which is better?

Advantages of Dependency Injection

- Using Dependency Injection
  - Removes hard coding of `new ClassName`
  - Creation is done outside class, so class only uses public API
  - Leads towards fewer assumptions in the code

Construction Patterns

Constructional Patterns

- Other methods include
  - See Gang of Four book
  - Strategy Pattern
  - Factory Pattern
  - Abstract Factory Pattern
  - Builder Pattern

- Also look up Service Locator Pattern

Managing Complexity

- Rather than monolithic code (bad)
- We end up with many smaller classes (good)
- So, its more flexible (good)
- But its more complex (bad)
- Who "owns" stuff?

Smart Pointers

Use of Raw Pointers

- Given a pointer passed to a function

```
void DoSomethingClever(int *a)
{
  // write some code
}
```

- How do we use the pointer?
- What problems are there?

Problems with Raw Pointers

- From "Effective Modern C++", Meyers, p117.
  - If you are done, do you destroy it?

- How to destroy it? Call `delete` or some method first: `a->Shutdown();`
- Single object or array?
- `delete` or `delete[]`?
- How to ensure the whole system only deletes it once?
- Is it dangling, if I don't delete it?

Use Smart Pointers

- `new/delete` on raw pointers not good enough
- So, use Smart Pointers
  - automatically delete pointed to object
  - explicit control over sharing
  - i.e. smarter
- Smart Pointers model the "ownership"

Further Reading

- Notes here are based on these:
  - David Kieras online paper
  - "Effective Modern C++", Meyers, ch4

Standard Library Smart Pointers

- Here we teach Standard Library
  - std::unique_ptr - models *has-a* but also unique ownership
  - std::shared_ptr - models *has-a* but shared ownership
  - std::weak_ptr - temporary reference, breaks circular references

Stack Allocated - No Leak.

- To recap:

```
#include "Fraction.h"
int main() {
  Fraction f(1,4);
}
```

- Gives:

```
I'm being deleted
```

- So stack allocated objects are deleted, when stack unwinds.

Heap Allocated - Leak.

- To recap:

```
#include "Fraction.h"
int main() {
  Fraction *f = new Fraction(1,4);
}
```

- Gives:

- So heap allocated objects are not deleted.
- Its the pointer (stack allocated) that's deleted.

Unique Ptr - Unique Ownership

- So:

```
#include "Fraction.h"
#include <memory>
int main() {
  std::unique_ptr<Fraction> f(new Fraction(1,4));
}
```

- Gives:

```
I'm being deleted
```

- And object is deleted.
- Is that it?

Unique Ptr - Move?

- Does move work?

```
#include "Fraction.h"
#include <memory>
#include <iostream>

int main() {
  std::unique_ptr<Fraction> f(new Fraction(1,4));
  // std::unique_ptr<Fraction> f2(f); // compile error

  std::cerr << "f=" << f.get() << std::endl;

  std::unique_ptr<Fraction> f2;
  // f2 = f; // compile error
  // f2.reset(f.get()); // bad idea

  f2.reset(f.release());
  std::cout << "f=" << f.get() << ", f2=" << f2.get() << std::endl;

  f = std::move(f2);
  std::cout << "f=" << f.get() << ", f2=" << f2.get() << std::endl;
}
```

- Gives:

```
f=0, f2=0x181e010
f=0x181e010, f2=0
I'm being deleted
```

- We see that API makes difficult to use incorrectly.

Unique Ptr - Usage 1

- Forces you to think about ownership
  - No copy constructor
  - No assignment
- Consequently
  - Can't pass pointer by value
  - Use move semantics for placing in containers

Unique Ptr - Usage 2

- Put raw pointer STRAIGHT into unique_ptr
- see `std::make_unique` in C++14.

```
#include "Fraction.h"
#include <memory>
int main() {
  std::unique_ptr<Fraction> f(new Fraction(1,4));
}
```

Shared Ptr - Shared Ownership

- Many pointers pointing to same object
- Object only deleted if no pointers refer to it
- Achieved via reference counting

Shared Ptr Control Block

- Won't go to too many details:

- From "Effective Modern C++", Meyers, p140

Shared Ptr - Usage 1

- Place raw pointer straight into shared_ptr
- Pass to functions, reference or by value
- Copy/Move constructors and assignment all implemented

Shared Ptr - Usage 2

```
#include "Fraction.h"
#include <memory>
#include <iostream>
void divideBy2(const std::shared_ptr<Fraction>& f)
{
  f->denominator *= 2;
}
void multiplyBy2(const std::shared_ptr<Fraction> f)
{
  f->numerator *= 2;
```

```
}
int main() {
  std::shared_ptr<Fraction> f1(new Fraction(1,4));
  std::shared_ptr<Fraction> f2 = f1;
  divideBy2(f1);
  multiplyBy2(f2);
  std::cout << "Value=" << f1->numerator << "/" << f1->denominator << std::endl;
  std::cout << "f1=" << f1.get() << ", f2=" << f2.get() << std::endl;
}
```

Shared Ptr - Usage 3

- Watch out for exceptions.
- "Effective Modern C++", Meyers, p140

```
#include "Fraction.h"
#include <memory>
#include <stdexcept>
#include <vector>
int checkSomething(const std::shared_ptr<Fraction>& f, const int& i)
{
  // whatever.
}
int computeSomethingFirst()
{
  // what if this throws?
}
int main()
{
  std::vector<std::shared_ptr<Fraction> >  spaceForLotsOfFractions;
  int result = checkSomething(std::shared_ptr<Fraction>(new Fraction(1,4)),
                              computeSomethingFirst()
                             );
}
```

Shared Ptr - Usage 4

- Prefer `std::make_shared`
- Exception safe

```
#include "Fraction.h"
#include <memory>
```

```
#include <stdexcept>
#include <vector>
int checkSomething(const std::shared_ptr<Fraction>& f, const int& i)
{
  // whatever.
}
int computeSomethingFirst()
{
  // what if this throws?
}
int main()
{
  std::vector<std::shared_ptr<Fraction> >  spaceForLotsOfFractions;
  int result = checkSomething(std::make_shared<Fraction>(1,4),
                              computeSomethingFirst()
                             );
}
```

Weak Ptr - Why?

- Like a shared pointer, but doesn't actually own anything
- Use for example:
  - Caches
  - Break circular pointers
- Limited API
- Not terribly common as most code ends up as hierarchies

Weak Ptr - Example

- See David Kieras online paper

```
#include "Fraction.h"
#include <memory>
#include <iostream>
int main() {
  std::shared_ptr<Fraction> s1(new Fraction(1,4));
  std::weak_ptr<Fraction> w1;      // can point to nothing
  std::weak_ptr<Fraction> w2 = s1; // assignment from shared
  std::weak_ptr<Fraction> w3(s1);  // construction from shared

  // Can't be de-referenced!!!
  // std::cerr << "Value=" << w1->numerator << "/" << w1->denominator << std::endl;
```

```
  // Needs converting to shared, and checking
  std::shared_ptr<Fraction> s2 = w1.lock();
  if (s2)
  {
    std::cout << "Object w1 exists=" << s2->numerator << "/" << s2->denominator << std::endl
  }

  // Or, create shared, check for exception
  std::shared_ptr<Fraction> s3(w2);
  std::cout << "Object must exists=" << s3->numerator << "/" << s3->denominator << std::endl
}
```

Final Advice

- Benefits of immediate, fine-grained, garbage collection
- Just ask Scott Meyers!
  - Use `unique_ptr` for unique ownership
  - Easy to convert `unique_ptr` to `shared_ptr`
  - But not the reverse
  - Use `shared_ptr` for shared resource management
  - Avoid raw `new` - use `make_shared`, `make_unique`
  - Use `weak_ptr` for pointers that can dangle (cache etc)

Comment on Boost

- Boost has become a sandbox for standard C++
- Boost features become part of standard C++, (different name space)
- So if you are forced to use old compiler
  - You could use boost - lecture 5.

Intrusive Vs Non-Intrusive

- Intrusive - Base class maintains a reference count eg. ITK
- Non-intrusive
  - `std::unique_ptr`
  - `std::shared_ptr`
  - `std::weak_ptr`
  - works for any class

ITK (intrusive) Smart Pointers

```
class MyFilter : // Other stuff
{
public:
  typedef MyFilter Self
  typedef SmartPointer<Self> Pointer;
  itkNewMacro(Self);
protected:
  MyFilter();
  virtual ~MyFilter();
};

double someFunction(MyFilter::Pointer p)
{
  // stuff
}

int main()
{
  MyFilter::Pointer p = itk::MyFilter::New();
}
```

Conclusion for Smart Pointers

- Default to standard library, check compiler
- Lots of other Smart Pointers
  - Boost (use STL).
  - ITK
  - VTK
  - Qt Smart Pointers
- Don't be tempted to write your own
- Always read the manual
- Always consistently use it

RAII Pattern

What is it?

- Resource Allocation Is Initialisation (RAII)
- Obtain all resources in constructor

- Release them all in destructor

Why is it?

- Guaranteed fully initialised object once constructor is complete
- Objects on stack are guaranteed to be destroyed when an exception is thrown and stack is unwound
  - Including smart pointers to objects

Example

- You may already be using it: STL example
- NifTK example
- Another example

Program To Interfaces

Why?

- In research code we often "just start hacking"
- You tend to mix interface and implementation
- Results in client of a class having implicit dependency on the implementation
- So, define a pure virtual class, not for inheritance, but for clean API

Example

```
#include <memory>
#include <vector>
#include <string>

class DataPlayerI {
public:
  virtual void StartPlaying() = 0;
  virtual void StopPlaying() = 0;
};

class FileDataPlayer : public DataPlayerI {
public:
  FileDataPlayer(const std::string& fileName){}; // opens file    (RAII)
```

```
  ~FileDataPlayer(){};                           // releases file (RAII)
public:
  virtual void StartPlaying() {};
  virtual void StopPlaying() {};
};

class Experiment {
public:
  Experiment(DataPlayerI *d) { m_Player.reset(d); } // takes ownership
  void Run() {};
  std::vector<std::string> GetResults() const {};
private:
  std::unique_ptr<DataPlayerI> m_Player;
};

int main(int argc, char** argv)
{
  FileDataPlayer fdp(argv[1]); // Or some class WebDataPlayer derived from DataPlayerI
  Experiment e(&fdp);
  e.Run();

  // etc.
}
```

Comments

- Useful between sub-components of a system
  - GUI front end, Web back end
  - Logic and Database
- Is useful in general to force loose connections between areas of code
  - e.g. different libraries that have different dependencies
  - e.g. camera calibration depends on OpenCV
  - define an interface that just exports standard types
  - stops the spread of dependencies
  - Lookup Pimpl idiom

Summary

All Together

- Program to interfaces

- Prefer composition over inheritance
- Inject dependencies
- Use constructional patterns to assemble code
- Always use smart pointers
- Always make fully initialised object
- Use exceptions for errors
- RAII very useful
- Results in a more flexible, extensible, robust design

Chapter 3

The Standard Template Library

The Standard Template Library

Contents

STL reference

- Containers
  - Sequences
  - Associative
- Iterators
- I/O streams
- Functors/functions
- Algorithms

Motivation

Motivation - why STL?

Because you have better things to do than rediscovering the wheel.

Task: Read in two files with an unknown number of integers, and sort them altogether.

The WRONG way to do it!

```
#include <stdio.h>
#include <stdlib.h>

int compare(const void* a, const void* b)
{
  return ( *(int*)a - *(int*)b );
}

int main()
{
  FILE* if1 = fopen("02stl/cpp/randomNumbers1.txt","r");
  FILE* if2 = fopen("02stl/cpp/randomNumbers2.txt","r");

  // First determine size of array needed
  int size1=0, size2=0;
  while (!feof(if1)) {
    fscanf(if1, "%*d");
    if (!feof(if1)) size1++;
  }
  rewind(if1);
  while (!feof(if2)) {
    fscanf(if2, "%*d");
    if (!feof(if2)) size2++;
  }
  rewind(if2);

  // Read in the data
  int theArray[size1+size2];
  for (int i=0;i<size1;++i) {
    fscanf(if1, "%d", &theArray[i]);
  }
  for (int i=size1;i<size1+size2;++i) {
    fscanf(if2, "%d", &theArray[i]);
  }
  fclose(if1);
  fclose(if2);

  // Sort and output
  qsort(theArray,size1+size2,sizeof(int),compare);
  for (int i=0;i<size1+size2;++i) {
    printf("%d ", theArray[i]);
  }
}
```

STL solution

```
#include <vector>
#include <algorithm>
#include <iostream>
#include <fstream>

int main()
{
  std::ifstream if1("02stl/cpp/randomNumbers1.txt",std::ifstream::in);
  std::ifstream if2("02stl/cpp/randomNumbers2.txt",std::ifstream::in);

  // Read in the data.
  int number;
  std::vector<int> theArray;
  while (!if1.eof()) {
    if1 >> number;
    if (!if1.eof()) theArray.push_back(number);
  }
  while (!if2.eof()) {
    if2 >> number;
    if (!if2.eof()) theArray.push_back(number);
  }
  if1.close();
  if2.close();

  // Sort and output
  std::sort(theArray.begin(),theArray.end());
  for (int i=0;i<theArray.size();++i) {
    std::cout << theArray[i] << " ";
  }
}
```

More conveniences

- Similar API between different STL containers. eg. myContainer->begin(), end(), at(), erase(), clear(), size(). . . ..
- Algorithms and data structures optimised for speed and memory.

STL Containers

Two general types:

- *Sequences*: Elements are ordered in a linear sequence. Individual elements are accessed by their position in this sequence/index. eg. `myVector[3]`, `myList.front()`, etc.
- *Associative*: Elements are referenced by their key and not by their position in the container. eg. `myMap['key1']`

Sequences

Properties:

- size: fixed/dynamic
- access: random/sequential
- underlying memory structure: contiguous/not
  - random access in non-contiguous memory is tricky
  - affects how efficiently inserting/removing of elements can be done
  - affects if pointer arithmetic can be done
- optimised insert/remove operations

Sequences

Name	size	access	memory	efficient insert/remove
array	fixed	random	contiguous	-
vector	**dynamic**	**random**	**contiguous**	**at end only**
deque	dynamic	random	non-contiguous	both ends
list	dynamic	sequential	non-contiguous	anywhere
forward_list	dynamic	sequential, only forward	non-contiguous	anywhere

More on vector

It's dynamic, so you can add/erase elements:

```
std::vector<int> myVec;
for (int i=0;i<10;++i) {
```

```
myVec.push_back(i);
}
myVec.insert(myVec.begin(),-1);
myVec.erase(1);
```

```
myVec = -1 1 2 3 4 5 6 7 8 9
```

. . . or manipulate its size:

```
std::vector<int> myVec(10);
std::cout << "Vector size before = " << myVec.size();
myVec.resize(5);
std::cout << " after = " << myVec.size() << "\n";
```

```
Vector size before = 10 after = 5
```

Note on C++11

- For all containers, `emplace(const_iterator position, Args&&... args)` is preferable to `insert(const_iterator position, const value_type& val)`, as it doesn't create any copies of the object you add to the container.
- Cases you might prefer something other than `emplace`:
  - backward compatibility
  - `insert` has more constructors
  - at least `emplace_back` might not work as expected in some implementations

Exercise

Think of cases where you'd use a specific container

Associative containers

Properties:

- key: is it separate from value?
  - maps: key-value pair
  - sets: value is the key (and thus it's const!)
- ordering. Affects performance:

  - unordered containers fastest to fill and access by key
  - ordered containers fastest to iterate through, and they're already ordered :o)
- unique values?

Associative containers

	ordered	unordered
unique	map	unordered_map
non-unique	multimap	unordered_multimap

	ordered	unordered
unique	set	unordered_set
non-unique	multiset	unordered_multiset

More on maps

Fill them with

```
std::map<std::string,int> myMap;
myMap["brocolli"] = 2;
myMap["garlic"] = 1;
myMap["brocolli"] = 1; // returns reference to element => element is updated
myMap.insert( std::pair<std::string,int>("bread",4) );
myMap.insert( std::pair<std::string,int>("brocolli",3) ); // returns iterator
                              // to existing element => element is not updated

typedef std::multimap<std::string,int> MMapType;
MMapType myMMap;                                    // there's no [] for multimap
myMMap.insert( std::pair<std::string,int>("brocolli",2) );
myMMap.insert( std::pair<std::string,int>("bread",4) );
myMMap.insert( std::pair<std::string,int>("brocolli",3) );
```

More on maps

Access elements with

```
  std::cout << "myMap[brocolli] = " << myMap["brocolli"] << "\n";
  std::cout << "myMap.find(bread) = " << myMap.find("bread")->second << "\n";
  for (std::map<std::string,int>::iterator it=myMap.begin(); it!=myMap.end(); ++it)
    std::cout << it->first << " " << it->second << "\n";

  std::cout << "myMMap.count(brocolli) = " << myMMap.count("brocolli") << "\n";
  std::pair < MMapType::iterator,MMapType::iterator> range = myMMap.equal_range("brocolli");
  for (MMapType::iterator it=range.first; it!=range.second; ++it)
    std::cout << it->first << " " << it->second << "\n";
  for (MMapType::iterator it=myMMap.begin(); it!=myMMap.end(); ++it)
    std::cout << it->first << " " << it->second << "\n";
```

```
myMap[brocolli] = 1
myMap.find(bread) = 4
bread 4
brocolli 1
garlic 1
myMMap.count(brocolli) = 2
brocolli 2
brocolli 3
bread 4
brocolli 2
brocolli 3
```

Example

Read in file with unknown number of particle-momentum pairs.

```
proton 4.5
electron 17.8
pion 4.6
muon 12.0
pion 3.2
neutrino 8.2
pion 23.7
proton 9.4
neutrino 6.7
```

- Then print out
  1. list of all particle-momentum pairs in alphabetical order
     – how about in ascending momentum order?
  2. list of types of particles in the file in alphabetical order
     – how about in mass order?
  3. list of particle-max momentum pairs

Task 1

```cpp
#include <map>
#include <string>
#include <iostream>
#include <fstream>

int main()
{
  std::ifstream ifs("02stl/cpp/particleList.txt",std::ifstream::in);
  // Read in the data
  std::multimap<std::string,double> theParticles;
  std::string name;
  double momentum;
  while (!ifs.eof()) {
    ifs >> name >> momentum;
    if (!ifs.eof())
      theParticles.insert( std::pair<std::string,double>(name,momentum) );
  }
  ifs.close();
  // Output - it's already sorted!
  std::multimap<std::string,double>::iterator iter = theParticles.begin();
  for ( ; iter!=theParticles.end(); ++iter) {
    std::cout << iter->first << " " << iter->second << std::endl;
  }
}
```

Task 2

- Hint1: use a set
- Hint2: write a custom comparator

Task 2

- Hint1: use a set
- Hint2: write a custom comparator

```cpp
class compMass {
public:
  compMass() :
    m_particlesOrdered({"neutrino", "electron", "muon", "pion", "kaon", "proton"})
  {};
  bool operator() (const std::string& s1, const std::string& s2) const
```

```
  {
    int index1=-1, index2=-1;
    for (int i=0;i<m_particlesOrdered.size();++i) {
      if (m_particlesOrdered[i]==s1) index1 = i;
      if (m_particlesOrdered[i]==s2) index2 = i;
    }
    return index1<index2; // unknown particles appear first (index=-1)
  }
private:
  std::vector<std::string> m_particlesOrdered;
};
```

then use it in the set constructor:

```
std::set<std::string,compMass> theParticles;
```

Task 3

Hint: extend the map class. - How?

- inherit from std::map - **NO**!
  - STL containers are *not* designed to be polymorphic, as they don't have virtual destructors (*Meyers 1:7*)
- composition - write a class that contains either an std::map object or smart pointer to it.
- free functions with STL containers/iterators as arguments

Task 3 - with function

```
void keepMax(std::map<std::string,double>& theMap, const std::string key, const double value
{
  if (theMap.find(key)==theMap.end()) //element doesn't already exist in map
    theMap[key] = value;
  else
    // any logic can go in here, eg a counter, an average, etc...
    theMap[key] = std::max(theMap[key],value);
}
```

Then use it in the loop when filling the container:

```
if (!feof(ifp)) keepMax( theParticles,name,momentum );
```

Task 3 - with composition

```
class maxMap
{
public:
  typedef std::map<std::string,double>::iterator iterator;

  void insert(const std::pair<std::string,double> theElement)
  {
    std::string key = theElement.first;
    double value = theElement.second;
    if (m_map.find(key)==m_map.end()) //element doesn't already exist in map
      m_map[key] = value;
    else
      // any logic can go in here, eg a counter, an average, etc...
      m_map[key] = std::max(m_map[key],value);
  }
  iterator begin() { return m_map.begin(); }
  iterator end() { return m_map.end(); }
private:
  std::map<std::string,double> m_map;
};
```

Task 3 - with composition

Then use it in main:

```
int main()
{
  std::ifstream ifs("02stl/cpp/particleList.txt",std::ifstream::in);
  // Read in the data
  maxMap theParticles;
  std::string name;
  double momentum;
  while (!ifs.eof()) {
    ifs >> name >> momentum;
    if (!ifs.eof())
      theParticles.insert( std::pair<std::string,double>(name,momentum) );
  }
  ifs.close();
  // Output - it's already sorted!
  maxMap::iterator iter = theParticles.begin();
  for ( ; iter!=theParticles.end(); ++iter) {
```

```
    std::cout << iter->first << " " << iter->second << std::endl;
  }
}
```

Accessing containers: iterators

For random-access containers you can do

```
std::vector<int> myVector = {1,2,3,4};
for (int i=0; i<myVector.size(); ++i) {
    std::cout << myVector[i] << std::endl;
}
```

But for sequential-access ones, you can only do

```
#include <iterator>

std::list<int> mylist = {1,2,3,4};
std::list<int>::iterator it=mylist.begin()
for ( ; it!=mylist.end(); ++it) {
    std::cout << *it << std::endl;
}
```

Iterators

An iterator is any object that, pointing to some element in a container, has the ability to iterate through the elements of that range using a set of operators.

- Minimum operators needed: increment (`++`) and dereference (`*`).
- A pointer is the simplest iterator.
- Brings some container-independence.
  - especially when using `typedef`

http://www.cplusplus.com/reference/iterator/

Pairs

```
#include <utility>      // std::pair
```

```
int main () {
  std::pair<std::string,double> product1;                     // default constructor
  std::pair<std::string,double> product2("tomatoes",2.30);   // value init

  auto foo = std::make_pair (10,20);                     // created a std::pair<int,int>
  product1 = std::make_pair(std::string("lightbulbs"),0.99);  // using make_pair

  product2.first = "shoes";                   // the type of first is string
  product2.second = 39.90;                    // the type of second is double

  std::cout << "foo: " << foo.first << ", " << foo.second << '\n';

  return 0;
}
```

Tuples

```
#include <tuple>        // std::tuple, std::make_tuple, std::get

int main()
{
  std::tuple<int,char> one;                          // default
  std::tuple<int,char> two(10,'a');                  // initialization

  auto first = std::make_tuple (10,'a');             // tuple < int, char >
  const int a = 0; int b[3];                         // decayed types:
  auto second = std::make_tuple (a,b);               // tuple < int, int* >

  std::cout << "two contains: " << std::get<0>(two);
  std::cout << " and " << std::get<1>(two);
  std::cout << std::endl;

  return 0;
}
```

Assignment

- Download a human genome file from ftp://ftp.ensembl.org/pub/release-87/fasta/homo_sapiens/dna/ . This is a sequence of characters from the dictionary {A,C,G,T,N}.
- List all the possible 3-letter combinations (k-mers for k=3) that appear in this file together with the number of appearances of each in the file, in

order of number of appearances.

  – Output should be something like

```
NNN 3345028
AGT 2348
CTT 1578
...
```

- Hint: use only associative containers. You'll need to extend their functionality to some kind of counter.

Other STL stuff

Contents

- I/O with streams
- Function objects
- Algorithms

Streams

- iostream for `std::cout`, `std::cerr` and `std::cin`
- fstream for file I/O
- sstream for string manipulation

```
std::ifstream myfile(filename,std::ifstream::in);
if (!myfile.good()) {
   stringstream mess;
   mess << "Cannot open file " << filename << " . It probably doesn't exist." << endl;
   throw runtime_error(mess.str());
}

myfile.seekg(0, std::ios::end);
m_size = myfile.tellg();
m_buffer = new char[m_size];
myfile.seekg(0, std::ios::beg);
myfile.read(m_buffer,m_size);
myfile.close();
```

Function objects

- Remember `std::set<std::string,compMass> theParticles;` ?
- There are several ways to define function-type stuff in c++, and `std::function` wraps them all
  - functions and function pointers
  - functors (i.e. an object with an `operator()` member function)
  - lambdas (i.e. nameless inline functions)
- Such functions can be used as comparators in STL containers or algorithms, among other things.

Function objects

```
#include <functional>   // std::function, std::negate

// a function:
int half(int x) {return x/2;}

// a function object class:
struct third_t {
  int operator()(int x) {return x/3;}
};

// a class with data members:
struct MyValue {
  int value;
  int fifth() {return value/5;}
};

int main () {
  std::function<int(int)> fn1 = half;                    // function
  std::function<int(int)> fn2 = &half;                   // function pointer
  std::function<int(int)> fn3 = third_t();               // function object
  std::function<int(int)> fn4 = [](int x){return x/4;};  // lambda expression
  std::function<int(int)> fn5 = std::negate<int>();      // standard function object

  std::cout << "fn1(60): " << fn1(60) << '\n';
  std::cout << "fn2(60): " << fn2(60) << '\n';
  std::cout << "fn3(60): " << fn3(60) << '\n';
  std::cout << "fn4(60): " << fn4(60) << '\n';
  std::cout << "fn5(60): " << fn5(60) << '\n';

  // stuff with members:
  std::function<int(MyValue&)> value = &MyValue::value;  // pointer to data member
```

```
  std::function<int(MyValue&)> fifth = &MyValue::fifth;  // pointer to member function

  MyValue sixty {60};
  std::cout << "value(sixty): " << value(sixty) << '\n';
  std::cout << "fifth(sixty): " << fifth(sixty) << '\n';
}
```

Function objects

Output:

```
fn1(60): 30
fn2(60): 30
fn3(60): 20
fn4(60): 15
fn5(60): -60
value(sixty): 60
fifth(sixty): 12
```

Algorithms

http://www.cplusplus.com/reference/algorithm/

- A collection of functions especially designed to be used on ranges of elements.
- Don't start coding any task, before checking if it's already there!

```
std::sort(RandomAccessIter first, RandomAccessIter last, Compare comp)

std::transform(InIter first, InIter last, OutIter res, UnaryOp op)
std::transform(InIter1 first1, InIter1 last1, InIter2 first2, OutIter res, BinaryOp op)

std::for_each (InIter first, InIter last, Function fn)

std::max_element(ForwardIter first, ForwardIter last, Compare comp)
std::min_element(ForwardIter first, ForwardIter last, Compare comp)
std::minmax_element(ForwardIter first, ForwardIter last, Compare comp)
```

Chapter 4

Libraries

Why use Libraries?

What are libraries?

- Libraries provide collections of useful classes and functions, ready to use.
- But code MUST be CORRECT for good science, so you need a good library.

Scientists perspective

- As a scientist you want:
  - Run experiments, demonstrate new concepts
  - To not spend too much time writing code, if its readily available.

Developers perspective

- As a developer:
  - You need to write some code yourself (as you're doing novel science)
  - But do you write all of it?

Our job as Craftsperson and Scholar necessitates knowledge of software engineering and science and to balance our usage of time.

Aim for this chapter

- How to choose a library
  - Licensing, longevity, developer community, technical implementation, feature list etc.
- Working with libraries
  - Illustrating C++ concepts, not an exhaustive product specific tutorial.

Choosing libraries

Libraries are awesome

A great set of libraries allows for a very powerful programming style:

- Write minimal code yourself
- Choose the right libraries
- Plug them together
- Create impressive results

Libraries for Efficiency

Not only is this efficient with your programming time, it's also more efficient with computer time.

The chances are any general algorithm you might want to use has already been programmed better by someone else.

Publihsing Results

CAVEAT: This is not legal advice. If in doubt, seek your own legal advice.

- If you use your code for internal use and you don't distribute it
  - then you are ok.
  - i.e. if 3rd party library wasn't for use, then it wouldn't be available.
  - you can publish results using open-source code
  - however, increasingly you are asked to share code . . . read on.

Distributing Software

CAVEAT: This is not legal advice. If in doubt, seek your own legal advice.

- However, you may plan to distribute your code:
  - Read this book, and/or GitHub's advice, and OSI for choosing your own license.
  - Don't write your own license, unless you use legal advice.
  - Try to pick one of the standard ones if you can, so your software is "compatible", and people understand the restrictions.

Choosing a License

- If you distribute your code, the licenses of any 3rd party libraries take effect:
  - MIT and BSD are permissive. So you can do what you want, including sell it on.
  - Apache handles multiple contributors and patent rights, but is basically permissive.
  - GPL requires you to open-source your code, including changes to the library you imported, and your work is considered a "derivative work", so must be shared.
  - LGPL for libraries, but use dynamic not static linkage. If you use static linking its basically as per GPL.

Note: Once a 3rd party has your code under a license agreement, their restrictions are determined by that version of the code.

Think Long Term

- On MPHYG001, we encouraged
  - Share your code, collaborate, take pride.
  - This improves your code and your science. (See this).
  - Your software should accumulate, reliably, and be extensible.

Choose Stability

- So, take care in your choice of 3rd party library
  - Don't want to redo work later, at the end of PhD.
  - Don't want to rely too heavily on non-distributable code.
  - But if you do, understand what that means.

Is Library Updated?

- Code that is not developed, rots.
  - When was the last commit?
  - How often are there commits?
  - Is the code on an open version control tool like GitHub?

Are Developers Reachable?

- Can you find the lead contributor on the internet?
  - Do they respond when approached?
- Are there contributors other than the lead contributor?

Is Code Tested?

- Are there many unit tests, do they run, do they pass?
- Does the library depend on other libraries?
- Are the build tools common?
- Is there a sensible versioning scheme (e.g. semantic versioning).
- Is there a suitable release schedule?

Library Quality

- Shouldn't need to look excessively closely, but consider
  - Documentation
  - Number of ToDo's
  - Dependencies
  - Data Structures? How to import/export image
  - Can you write a convenient wrapper?

Library Features

- Then look at features
  - Manual
  - Easy to use

Summary

- In comparison with languages such as Python
  - In C++ prefer few well chosen libraries
  - Be aware of their licenses for future distribution
  - Keep a log of any changes, patches etc. that you make
  - Be able to compile all your own code, including libraries
    * so need common build environment. (eg. CMake, Make, Visual Studio).

Linking libraries

Aim

- Can be difficult to include a C++ library
- Step through
  - Dynamic versus Static linking
- Aim for - source code based distribution

Linking

- Code is split into functions/classes
- Related functions get grouped into libraries
- Libraries have namespaces, names, declaration, definitions (implementations)
- Libraries get compiled - saves compilation time
- End User needs
  - Header file = declarations
  - Object code / library file = implementations

Static Linking

- Windows (.lib), Mac/Linux (.a)
- Compiled code from static library is copied into the current translation unit.
- Increases disk space
- Current translation unit then does not depend on that library.

Dynamic Linking

- Windows (.dll), Mac (.dylib), Linux (.so)
- Compiled code is left in the library.
- At runtime,
  - OS loads the executable
  - Finds any unresolved libraries
    - Various search mechanisms
  - Recursive process
- Saves disk space
- Current translation unit has a known dependency remaining.

Dynamic Loading

- System call to load a library (dlopen/LoadLibrary)
- Dynamically discover function names and variables
- Execute functions
- Normally used for plugins
- Not covered here

Space Comparison

- If you have many executables linking a common set of libraries
- Static
  - Code gets copied - each executable bigger
  - Doesn't require searching for libraries at run-time
- Dynamic
  - Code gets referenced - smaller executable
  - Requires finding libraries at run-time
- Less of a concern these days

How to Check

- Windows - Dependency Walker
- Linux - `ldd`
- Mac - `otool -L`
- (live demo on Mac)

Note about Licenses

CAVEAT: Again - this is not legal advice.

- Static linking considered to make your work a 'derivative work'
- If you use LGPL - use dynamic linking

Using libraries

Aim

- Can be difficult to include a C++ library
- Step through
  - Build structure
- Aim for - source code based distribution

Where from?

- Package Manager (Linux/Mac)
  - Precompiled
  - Stable choice
  - Inter-dependencies work
- For example
  - `sudo apt-get install`
  - `port install`
  - `brew install`

Windows

- Libraries typically:
  - Randomly installed location
  - In system folders
  - In developer folders
  - In build folder
- Package managers forthcoming

Problems

- As soon as you hit a bug in a library
  - How to update?
  - Knock on effects
    * Cascading updates
    * Inconsistent development environment

External Build

- 2 basic approaches
  - Separate build
    * Build dependencies externally
    * Point your software at those packages

Example

For example

```
C:\build\ITK
C:\build\ITK-build
C:\build\ITK-install
C:\build\VTK
C:\build\VTK-build
C:\build\VTK-install
C:\build\MyProject
C:\build\MyProject-build
```

We setup `MyProject-build` to know the location of ITK and VTK.

Meta-Build

- 2 basic approaches
  - Meta-Build, a.k.a SuperBuild
    * Your software coordinates building dependencies

Example

For example

```
C:\build\MyProject
C:\build\MyProject-SuperBuild\ITK\src
C:\build\MyProject-SuperBuild\ITK\build
C:\build\MyProject-SuperBuild\ITK\install
C:\build\MyProject-SuperBuild\VTK\src
C:\build\MyProject-SuperBuild\VTK\build
C:\build\MyProject-SuperBuild\VTK\install
C:\build\MyProject-SuperBuild\MyProject-build
```

We setup `MyProject-build` to know the location of ITK and VTK.

Including libraries

Aim

- Can be difficult to include a C++ library
- Step through
  - Ways of setting paths/library names
    - Platform specific
    - Use of CMake
- Aim for - source code based distribution

Recap

- So far
  - Seen how to chose
  - Static / Dynamic
  - How to structure layout
- Now we want to use a library

Fundamental

- Access to header files - declaration
- Access to compiled code - definition

Linux/Mac

```
g++ -c -I/users/me/myproject/include main.cpp
g++ -o main main.o -L/users/me/myproject/lib -lmylib
```

- `-I` to specify include folder
- `-L` to specify library folder
- `-l` to specify the actual library

Notice: you don't specify .a or .so/.dylib if only 1 type exists.

Windows

- Visual Studio (check version)
- Project Properties
  - C/C++ -> Additional Include Directories.
  - Configuration Properties -> Linker -> Additional Library Directories
  - Linker -> Input -> Additional Dependencies.
- Check compile line - its equivalent to Linux/Mac, -I, -L, -l

Header Only?

- After all this:
  - Static/Dynamic
  - Package Managers / Build your own
  - External build / Internal Build
  - Release / Debug
  - -I, -L, -l
- Header only libraries are very attractive.

Use of CMake

- Several ways depending on your setup
  - Hard code paths and library names
  - Use a FindModule
  - Generate and use a FindModule

CMake - Header Only

- catch.hpp Header files in project CMakeCatchTemplate
- From `CMakeCatchTemplate/CMakeLists.txt`

```
include_directories(${CMAKE_SOURCE_DIR}/Code/)
add_subdirectory(Code)
if(BUILD_TESTING)
  include_directories(${CMAKE_SOURCE_DIR}/Testing/)
  add_subdirectory(Testing)
endif()
```

CMake - Header Only

- Options are:
  - Check small/medium size project into your project
- For example:

  ```
  CMakeCatchTemplate/3rdParty/libraryA/version1/Class1.hpp
  CMakeCatchTemplate/3rdParty/libraryA/version1/Class2.hpp
  ```

- Add to CMakeLists.txt

  ```
  include_directories(${CMAKE_SOURCE_DIR}/3rdParty/libraryA/version1/)
  ```

- You'd have audit trail (via git repo) of when updates to library were made.

CMake - Header Only External

- If larger, e.g. Eigen

```
C:\3rdParty\Eigen
C:\build\MyProject
C:\build\MyProject-build
```

- Add to CMakeLists.txt

  ```
  include_directories("C:\3rdParty\Eigen\install\include\eigen3\
  ```

- Hard-coded, but usable if you write detailed build instructions
- Not very platform independent
- Not very flexible
- Can be self contained if you have a Meta-build

CMake - find_package

- For example:

```
find_package(OpenCV REQUIRED)
include_directories(${OpenCV_INCLUDE_DIRS})
list(APPEND ALL_THIRD_PARTY_LIBRARIES ${OpenCV_LIBS})
add_definitions(-DBUILD_OpenCV)
```

- So a package can provide information on how you should use it
- If its written in CMake code, even better!

find_package - Intro

- CMake comes with scripts to include 3rd Party Libraries
- You can also write your own ones

find_package - Search Locations

A Basic Example (for a full example - see docs)

- Given:

```
find_package(SomeLibrary [REQUIRED])
```

- CMake will search
  - all directories in CMAKE_MODULE_PATH
  - for FindSomeLibrary.cmake
  - case sensitive

find_package - Result

- If file is found, CMake will try to run it, to find that library.
- FindSomeLibrary.cmake should return SomeLibrary_FOUND:BOOL=TRUE if library was found
- Sets any other variables necessary to use the library
- Check CMakeCache.txt

find_package - Usage

- So many 3rd party libraries are CMake ready.
- If things go wrong, you can debug it - not compiled

find_package - Fixing

- You can provide patched versions
- Add your source/build folder to the CMAKE_MODULE_PATH

```
set(CMAKE_MODULE_PATH
    ${CMAKE_SOURCE_DIR}/CMake
    ${CMAKE_BINARY_DIR}
    ${CMAKE_MODULE_PATH}
   )
```

- So CMake will find your version before the system versions

find_package - Tailoring

- You can write your own
  - e.g. FindEigen in CMakeCatchTemplate
- Use CMake to substitute variables
  - Force include/library dirs
  - Useful for vendors API that isn't CMake compatible
  - Useful for meta-build. Force directories to match the package you just compiled.

Provide Build Flags

- If a package is found, you can add compiler flag.

```
add_definitions(-DBUILD_OpenCV)
```

- So, you can optionally include things:

```
#ifdef BUILD_OpenCV
#include <cv.h>
#endif
```

- Best not to do too much of this.
- Useful to provide build options, e.g. for running on clusters

Check Before Committing

- Before you commit code to git,
- Make sure you are compiling what you think you are!

```
#ifdef BUILD_OpenCV
blah blah
#include <cv.h>
#endif
```

- should fail compilation

Summary

- Basic aim:
  - `include_directories()` generates -I
  - ‘`link_directories()` generates -L
  - `target_link_libraries(mylibrary PRIVATE ${libs})` generates -l for each library
- Might not need `link_directories()` if libraries fully qualified
- Try default CMake find_package
- Or write your own and add location to CMAKE_MODULE_PATH

Using Eigen

Introduction

- Eigen is:
  - C++ template library,
  - Linear algebra, matrices, vectors, numerical solvers, etc.
  -

Module	Header file	Contents
Core	`#include <Eigen/Core>`	Matrix and Array classes, basic linear algebra (including triangular and selfadjoint products), array manipulation
Geometry	`#include <Eigen/Geometry>`	Transform, Translation, Scaling, Rotation2D and 3D rotations (Quaternion, AngleAxis)
LU	`#include <Eigen/LU>`	Inverse, determinant, LU decompositions with solver (FullPivLU, PartialPivLU)
Cholesky	`#include <Eigen/Cholesky>`	LLT and LDLT Cholesky factorization with solver
Householder	`#include <Eigen/Householder>`	Householder transformations; this module is used by several linear algebra modules
SVD	`#include <Eigen/SVD>`	SVD decomposition with least-squares solver (JacobiSVD)
QR	`#include <Eigen/QR>`	QR decomposition with solver (HouseholderQR, ColPivHouseholderQR, FullPivHouseholderQR)
Eigenvalues	`#include <Eigen/Eigenvalues>`	Eigenvalue, eigenvector decompositions (EigenSolver, SelfAdjointEigenSolver, ComplexEigenSolver)
Sparse	`#include <Eigen/Sparse>`	Sparse matrix storage and related basic linear algebra (SparseMatrix, DynamicSparseMatrix, SparseVector)
	`#include <Eigen/Dense>`	Includes Core, Geometry, LU, Cholesky, SVD, QR, and Eigenvalues header files
	`#include <Eigen/Eigen>`	Includes Dense and Sparse header files (the whole Eigen library)

Tutorials

Obviously, you can read:

- the existing manual pages
- tutorials (short, long).
- the Quick Reference

Getting started

- Header only, just need `#include`
- Uses CMake, but that's just for
  - documentation
  - run unit tests
  - do installation.

C++ Principles

(i.e. why introduce Eigen on this course)

- Eigen uses
  - Templates
  - Loop unrolling, traits, template meta programming

Matrix Class

- This:

```
#include <iostream>
#include <Eigen/Dense>
using Eigen::MatrixXd;
int main()
{
  MatrixXd m(2,2);
  m(0,0) = 3;
  m(1,0) = 2.5;
  m(0,1) = -1;
  m(1,1) = m(1,0) + m(0,1);
  std::cout << m << std::endl;
}
```

- Produces:

```
  3  -1
2.5 1.5
```

Matrix Class Declaration

Matrix Class

```
template<typename _Scalar, int _Rows, int _Cols, int _Options, int _MaxRows, int _MaxCols>
class Matrix
  : public PlainObjectBase<Matrix<_Scalar, _Rows, _Cols, _Options, _MaxRows, _MaxCols> >
{
```

So, its templates, so review last weeks lecture.

Matrix Class Construction

But in documentation:

All combinations are allowed: you can have a matrix with a fixed number of rows and a dynamic number of columns, e
are all valid:

```
Matrix<double, 6, Dynamic>                  // Dynamic number of columns (heap allocation)
Matrix<double, Dynamic, 2>                  // Dynamic number of rows (heap allocation)
Matrix<double, Dynamic, Dynamic, RowMajor>  // Fully dynamic, row major (heap allocation)
Matrix<double, 13, 3>                       // Fully fixed (usually allocated on stack)
```

Figure 4.1: Matrix construction

It took a while but I searched and found:

```
src/Core/util/Constants.h:const int Dynamic = -1;
```

and both fixed and dynamic Matrices come from same template class???

How do they do that?

DenseStorage.h - 1

In `src/Core/DenseStorage.h`:

```
template <typename T, int Size, int MatrixOrArrayOptions,
          int Alignment = (MatrixOrArrayOptions&DontAlign) ? 0
                          : (((Size*sizeof(T))%16)==0) ? 16
                          : 0 >
struct plain_array
{
  T array[Size];
```

So, a `plain_array` structure containing a stack allocated array.

DenseStorage.h - 2

In `src/Core/DenseStorage.h`:

```
// purely fixed-size matrix
template<typename T, int Size, int _Rows, int _Cols, int _Options> class DenseStorage
{
    internal::plain_array<T,Size,_Options> m_data;
```

There is a default template class for DenseStorage, and specialisation for fixed arrays.

DenseStorage.h - 3

In `src/Core/DenseStorage.h`:

```
// purely dynamic matrix.
template<typename T, int _Options> class DenseStorage<T, Dynamic, Dynamic, Dynamic, _Options
{
    T *m_data;
    DenseIndex m_rows;
    DenseIndex m_cols;
```

There is a default template class for DenseStorage, and specialisation for Dynamic arrays.

Eigen Matrix Summary

- Templated type supports dynamic and fixed arrays seamlessly on stack or heap
- typedef's to make life easier: `Matrix3d` = 3 by 3 of double

- Uses TMP to generate generate code at compile time
- Benefit from optimisations such as loop unrolling when using fixed size constant arrays

Eigen Usage - CMake Include

- Need to set include path
- You could download and 'install' eigen into your project, and commit it. e.g.

```
include_directories(${CMAKE_SOURCE_DIR}/session03/cpp/Eigen/eigen-3.2.3/include/eigen3)
```

Eigen Usage - CMake Module

- CMake (3.1) does not have a `Find Module` for eigen, but eigen provides one.
- So, in your source tree

```
mkdir CMake
cp <path_to_eigen>/cmake/FindEigen3.cmake ./CMake
```

- Then in your CMakeLists.txt

```
set(CMAKE_MODULE_PATH "${CMAKE_SOURCE_DIR}/CMake;${CMAKE_MODULE_PATH}")
find_package(Eigen3)
include_directories(${EIGEN3_INCLUDE_DIR})
```

Eigen Usage - CMake External

- NiftySeg uses

```
option(USE_SYSTEM_EIGEN "Use an already installed version of the Eigen library" OFF)
if(USE_SYSTEM_EIGEN)
  find_package(EIGEN REQUIRED)
else()
  set(${PROJECT_NAME}_VERSION_EIGEN "ffa86ffb5570" CACHE STRING "Version of EIGEN" FORCE)
  set(${PROJECT_NAME}_MD5_SUM_EIGEN 9559c34af203dde5f3f1d976d859c5b3 CACHE STRING "MD5 check
  set(${PROJECT_NAME}_LOCATION_EIGEN
    "http://cmic.cs.ucl.ac.uk/platform/dependencies/eigen-eigen-${${PROJECT_NAME}_VERSION_E
    CACHE STRING "Location of Eigen" FORCE)
  ExternalProject_Add(Eigen
    URL ${${PROJECT_NAME}_LOCATION_EIGEN}
```

```
    URL_MD5 ${${PROJECT_NAME}_MD5_SUM_EIGEN}
    PREFIX ${PROJECT_BINARY_DIR}/Eigen
    DOWNLOAD_DIR ${PROJECT_BINARY_DIR}/Eigen/download
    SOURCE_DIR ${PROJECT_BINARY_DIR}/Eigen/source
    STAMP_DIR ${PROJECT_BINARY_DIR}/Eigen/stamps
    TMP_DIR ${PROJECT_BINARY_DIR}/Eigen/tmp
    BINARY_DIR ${PROJECT_BINARY_DIR}/Eigen/build
    CMAKE_ARGS
      ${CMAKE_PROPAGATED_VARIABLES}
      -DCMAKE_INSTALL_PREFIX:PATH=${PROJECT_BINARY_DIR}/Eigen/install
      -DBUILD_TESTING=1
    )
  set(Eigen_INCLUDE_DIR ${PROJECT_BINARY_DIR}/Eigen/install/include/eigen3)
endif()
include_directories(${Eigen_INCLUDE_DIR})
```

Eigen Example - in PCL

Point Cloud Library uses Eigen. Lets look at point based registration of two, same length, point sets.

PCL - Manual Registration

- Class to hold point lists
- Callbacks (not shown here) to add points to list

```
class ManualRegistration : public QMainWindow
{
  protected:
  pcl::PointCloud<pcl::PointXYZ>    src_pc_;
  pcl::PointCloud<pcl::PointXYZ>    dst_pc_;
  Eigen::Matrix4f                   transform_;
```

PCL - SVD class

- In `apps/src/manual_registration/manual_registration.cpp`
- Create a class to estimate SVD of two point sets
- See paper Arun et. al. 1987
- Its an example of the orthogonal procrustes problem

```
  pcl::registration::TransformationEstimationSVD<pcl::PointXYZ, pcl::PointXYZ> tfe;
  tfe.estimateRigidTransformation(src_pc_, dst_pc_, transform_);
```

PCL - Correlation

After subtracting each point from the mean point we have in `registration/include/pcl/registration/impl/t`

```
template <typename PointSource, typename PointTarget, typename Scalar> void
pcl::registration::TransformationEstimationSVD<PointSource, PointTarget, Scalar>::getTransfo
    const Eigen::Matrix<Scalar, Eigen::Dynamic, Eigen::Dynamic> &cloud_src_demean,
    const Eigen::Matrix<Scalar, 4, 1> &centroid_src,
    const Eigen::Matrix<Scalar, Eigen::Dynamic, Eigen::Dynamic> &cloud_tgt_demean,
    const Eigen::Matrix<Scalar, 4, 1> &centroid_tgt,
    Matrix4 &transformation_matrix) const
{
  transformation_matrix.setIdentity ();

  // Assemble the correlation matrix H = source * target'
  Eigen::Matrix<Scalar, 3, 3> H = (cloud_src_demean * cloud_tgt_demean.transpose ()).topLeft

  // Compute the Singular Value Decomposition
  Eigen::JacobiSVD<Eigen::Matrix<Scalar, 3, 3> > svd (H, Eigen::ComputeFullU | Eigen::Comput
  Eigen::Matrix<Scalar, 3, 3> u = svd.matrixU ();
  Eigen::Matrix<Scalar, 3, 3> v = svd.matrixV ();

  // Compute R = V * U'
  if (u.determinant () * v.determinant () < 0)
  {
    for (int x = 0; x < 3; ++x)
      v (x, 2) *= -1;
  }

  Eigen::Matrix<Scalar, 3, 3> R = v * u.transpose ();

  // Return the correct transformation
  transformation_matrix.topLeftCorner (3, 3) = R;
  const Eigen::Matrix<Scalar, 3, 1> Rc (R * centroid_src.head (3));
  transformation_matrix.block (0, 3, 3, 1) = centroid_tgt.head (3) - Rc;
}
```

PCL - Summary

- Use of Eigen implements Arun et. al. 1987 in one main function.
- Relatively close matching of algorithm to code.
- Template notation a bit awkward, but now, not so insurmountable.
- So, using library, we gain power and benefit of very experienced library programmers.

Eigen Summary

- Header only
- Use CMake to set the include path
- Templated, so its compiled in, no link or run-time dependencies
- Simple to use linear algebra library
- Advise not to mix with GUI code
- Consider static linking as using templates anyway - ease of distribution

Using Boost

Introduction

- Boost is "…one of the most highly regarded and expertly designed C++ library projects in the world."
- A large (121+) collection of C++ libraries
- Aim to establish standards, contribute to C++11, C++17 etc.
- Hard to use C++ without bumping into Boost at some point
- It's heavily templated
- Many libraries header only, some require compiling.

Libraries included

- Log, FileSystem, Asio, Serialization, Pool (memory) …
- Regexp, String Algo, DateTime, …
- Math, Odeint, Graph, Polygon, Rational, …
- Each has good documentation, and tutorial, and unit tests, and is widely compiled.

Getting started

- Default build system: `bjam`
- Also CMake version of boost project, possible deprecated.
- Once installed, many header only libraries, so similar to Eigen.

Installing pre-compiled

- Linux:
  - `sudo apt-get install boost`
  - `sudo apt-get install libboost1.53-dev`

- Mac
  - Homebrew (brew) or Macports (port)
- Windows
  - Precompiled binaries? Probably you need to build from source.

Compiling from source

- Follow build instructions here
- Or use bigger project with it as part of build system
  - NifTK, MITK, Slicer, Gimias (medical imaging)

C++ Principles

(i.e. why introduce Boost on this course)

- Boost uses
  - Templates
  - Widespread use of:
    * Generic Programming
    * Template Meta-Programming
  - Functors

C Function Pointers - 1

- Useful if using Numerical Recipes in C
- See Wikipedia article and tutorials online

This:

```
#include <stdio.h>  /* for printf */
double cm_to_inches(double cm) {
  return cm / 2.54;
}
int main(void) {
  double (*func1)(double)            = cm_to_inches;
  printf("Converting %f cm to %f inches by calling function.\n", 5.0, cm_to_inches(5.0));
  printf("Converting %f cm to %f inches by deref pointer.\n", 15.0, func1(15.0));
  return 0;
}
```

Produces:

```
Converting 5.000000 cm to 1.968504 inches by calling function.
Converting 15.000000 cm to 5.905512 inches by deref pointer.
```

C Function Pointers - 2

- Function pointers can be passed to functions

This:

```c
#include <stdio.h>
#include <math.h>
double integrate(double (*funcp)(double), double lo, double hi) {
  double  sum = 0.0;
  for (int i = 0;  i <= 100;  i++)
  {
    sum += (*funcp)(i / 100.0 * (hi - lo) + lo);
  }
  return sum / 100.0;
}
int main(void) {
  double  (*fp)(double) = sin;
  printf("sum(sin): %f\n", integrate(fp, 0.0, 1.0));
  return 0;
}
```

Produces:

```
sum(sin): 0.463901
```

C Function Pointers - 3

- Function pointers
  - often used for callbacks, cost functions in optimisation etc.
  - called by name, or dereference pointer
  - are generally stateless

C++ Function Objects - 1

- We can define an object to represent a function
  - Called Function Object or Functor

This:

```
#include <vector>
#include <algorithm>
#include <iostream>
struct IntComparator
{
  bool operator()(const int &a, const int &b) const
  {
    return a < b;
  }
};
/*
template <class RandomIt, class Compare>
void sort(RandomIt first, RandomIt last, Compare comp);
*/
int main()
{
    std::vector<int> items;
    items.push_back(1);
    items.push_back(3);
    items.push_back(2);
    std::sort(items.begin(), items.end(), IntComparator());
    std::cout << items[0] << "," << items[1] << "," << items[2] << std::endl;
    return 0;
}
```

Produces:

```
1,2,3
```

C++ Function Objects - 2

- But function objects can
  - Have state
  - Have member variables
  - Be complex objects, created by any means
  - e.g. Cost function, similarity between two images

CMake for Boost

- If installed correctly, should be something like:

```
set(Boost_ADDITIONAL_VERSIONS 1.53.0 1.54.0 1.53 1.54)
find_package(Boost 1.53.0)
if(Boost_FOUND)
    include_directories(${Boost_INCLUDE_DIRS})
endif()
```

Boost Example

- With 121+ libraries, can't give tutorial on each one!
- Pick one small numerical example
- Illustrate the use of functors in ODE integration

Using Boost odeint

- Its a numerical example, as we are doing scientific computing!
- As with many libraries, just include right header

```
#include <boost/numeric/odeint.hpp> // Include ODE solver library
                                    // just to check our build system found it
```

- See this tutorial

Boost odeint - 1

Given these global definitions:

```
const double gam = 0.15;
typedef std::vector< double > state_type;

// This is functor class
```

Boost odeint - 2

First define a functor for the function to integrate:

```
class harm_osc {
    double m_gam; // class can have member variables, state etc.
public:
    harm_osc( double gam ) : m_gam(gam) { }

    // odeint integrators normally call f(x, dxdt, t)
    void operator() ( const state_type &x , state_type &dxdt , const double /* t */ )
    {
        dxdt[0] = x[1];
        dxdt[1] = -x[0] - m_gam*x[1];
    }
};

// This is observer to record output, and is also a functor class
```

Boost odeint - 3

Define an observer to collect graph-points:

```
struct push_back_state_and_time
{
    std::vector< state_type >& m_states;
    std::vector< double >& m_times;

    push_back_state_and_time( std::vector< state_type > &states , std::vector< double > &tim
    : m_states( states ) , m_times( times ) { }

    void operator()( const state_type &x , double t )
    {
        m_states.push_back( x );
        m_times.push_back( t );
    }
};
```

Boost odeint - 4

The run it:

```
int main(void) {

  state_type x(2);
```

```
  x[0] = 1.0; // start at x=1.0, p=0.0
  x[1] = 0.0;

  std::vector<state_type> x_vec; // vector of vectors
  std::vector<double> times;     // stores each time point

  harm_osc harmonic_oscillator(0.15);
  size_t steps = boost::numeric::odeint::integrate(
    harmonic_oscillator ,
    x , 0.0 , 10.0 , 0.1 ,
    push_back_state_and_time( x_vec , times ) );

  for( size_t i=0; i<=steps; i++ )
  {
    std::cout << times[i] << '\t' << x_vec[i][0] << '\t' << x_vec[i][1] << '\n';
  }

}
```

Boost odeint - 4

Produces:

```
0   1   0
0.1 0.995029    -0.0990884
0.342911    0.942763    -0.32773
0.59639 0.832373    -0.537274
0.865439    0.662854    -0.714058
1.15445 0.436595    -0.839871
1.44346 0.184494    -0.892171
1.70128 -0.0446646  -0.875731
1.9591  -0.262234   -0.80313
2.21692 -0.454545   -0.681207
2.48815 -0.616993   -0.510476
2.77613 -0.733844   -0.296963
3.06411 -0.7866 -0.0685387
3.35209 -0.773719   0.155753
3.64008 -0.699015   0.358007
3.92806 -0.571123   0.522852
4.21604 -0.402601   0.638582
4.50402 -0.20875    0.697943
4.792   -0.0062679  0.698535
5.07998 0.188159    0.642795
5.36797 0.359199    0.537596
5.65595 0.494053    0.39351
```

```
5.94393 0.583381    0.223796
6.23191 0.621907    0.0432166
6.51989 0.608673    -0.133212
6.80787 0.546935    -0.291443
7.09586 0.44372 -0.419492
7.39491 0.303457    -0.510857
7.69397 0.143005    -0.553869
7.99302 -0.0228226  -0.546913
8.29208 -0.179394   -0.492786
8.59113 -0.313525   -0.398255
8.89019 -0.414555   -0.273299
9.18925 -0.475166   -0.130101
9.4883  -0.49187    0.0181101
9.78736 -0.465143   0.158247
10  -0.421907   0.246407
```

Why Boost for Numerics

- Broader question is
  - Why someone else's library? Boost or some other.
- Advanced use of Template Meta Programming, Traits
  - Performance optimisations
  - Alternative implementations
    - CUDA via Thrust
    - MPI
    - etc
- You just focus on your bit

Using ITK

Introduction

- Insight Segmentation and Registration Toolkit
- Insight Journal for library additions
- Large community in medical image processing
- Deliberately no visualisation, see VTK.

C++ Principles

- Heavy use of Generic Programming

- Use of Template Meta-Programming
- Often perceived by "scientific programmers" (Matlab) as difficult
- Aim: demonstrate here, that we can now use it!
- Of particular interest
  - typedefs - make life easier
  - SmartPointers - reduce leaking memory
  - Iterators - fast image access
  - Object Factories - extensibility

Architecture Concept

- Use of pipeline of filters
- Simple to plug image processing filters together
- Sometimes difficult to manage memory for huge images

Filter Usage - 1

We work through a simple filter program. First, typedefs are aliases.

```
int main(int argc, char** argv)
{

  const unsigned int Dimension = 2;
  typedef int PixelType;
  typedef itk::Image<PixelType, Dimension> ImageType;
  typedef itk::AddImageFilter<ImageType, ImageType> AddFilterType;
  typedef itk::ImageFileReader<ImageType> ImageReaderType;
  typedef itk::ImageFileWriter<ImageType> ImageWriterType;
```

Filter Usage - 2

Objects are constructed:

```
  ImageReaderType::Pointer reader1 = ImageReaderType::New();
  ImageReaderType::Pointer reader2 = ImageReaderType::New();
  AddFilterType::Pointer addFilter = AddFilterType::New();
  ImageWriterType::Pointer writer = ImageWriterType::New();

  // eg. if not using typedefs
  //itk::ImageFileWriter< itk::Image<int, 2> >::Pointer writer
  //  = itk::ImageFileWriter< itk::Image<int, 2> >::New();
```

Filter Usage - 3

Pipeline is executed:

```
  reader1->SetFileName("inputFileName1.nii");
  reader2->SetFileName("inputFileName2.nii");
  addFilter->SetInput(0, reader1->GetOutput());
  addFilter->SetInput(1, reader2->GetOutput());
  writer->SetInput(addFilter->GetOutput());
  writer->SetFileName("outputFileName1.nii");
  //writer->Update(); // commented out, as filenames are fake.
                      // and build system for lecture notes
                      // tries to run the program.
  return 0;
}
```

More information on ITK Pipeline can be found in the ITK Software Guide.

Smart Pointer Intro

Lets look at some interesting features.

- Smart Pointer
  - Class, like a pointer, but 'Smarter' (clever)
  - Typically, once allocated will automatically destroy the pointed to object
  - Implementations vary, STL, ITK, VTK, Qt, so read the docs
- So, in each class e.g. itkAddImageFilter

```
typedef AddImageFilter     Self
typedef SmartPointer<Self> Pointer
```

and so, its used like

```
ClassName::Pointer variableName = ClassName::New();
```

Smart Pointer Class

In the SmartPointer itself

```
  /** Constructor to pointer p  */
  SmartPointer (ObjectType *p):
    m_Pointer(p)
  { this->Register(); }

  /** Destructor  */
  ~SmartPointer ()
  {
    this->UnRegister();
    m_Pointer = ITK_SP_NULLPTR;
  }
```

and

```
private:
  /** The pointer to the object referred to by this smart pointer. */
  ObjectType *m_Pointer;

  void Register()
  {
    if ( m_Pointer ) { m_Pointer->Register(); }
  }
```

General Smart Pointer Usage

- Avoid use of explicit pairs of `new/delete`
- Immediately assign object to SmartPointer
- Consistently (i.e. always) use SmartPointer
  - Pass (reference to) SmartPointer to function.
  - Can (but should you?) return SmartPointer from function.
  - Don't use raw pointer, and don't store raw pointers to objects.
  - You can't test raw pointer to check if object still exists.
- Object is deleted when last SmartPointer reference goes out of scope

ITK SmartPointer

- ITK keeps reference count in itk::LightObject base class
- So, it can only be used by sub-classes of itk::LightObject
- Reference is held in the object
- Same method used in MITK, as MITK uses ITK concepts
- VTK has a SmartPointer that requires calling Delete explicitly (!!)
- STL has much clearer definition of different types of smart pointer
- Read THIS tutorial

Implementing a Filter

- ITK provides many image processing filters.
- But you can write your own easily
  - Single Threaded - override GenerateData()
  - Multi-Threaded - override ThreadedGenerateData()
- Now we see an example - thresholding, as we want to study the C++ not the image processing.

Filter Impl - 1

Basic filter:

```
namespace itk
{
template< class TInputImage, class TOutputImage = TInputImage>
class MyThresholdFilter:public ImageToImageFilter< TInputImage, TOutputImage >
{
public:
```

Filter Impl - 2

Boilerplate nested typedefs :

```
  /** Standard class typedefs. */
  typedef MyThresholdFilter                                 Self;
  typedef ImageToImageFilter< TInputImage, TOutputImage > Superclass;
  typedef SmartPointer< Self >                              Pointer;
  typedef typename TInputImage::PixelType                   InputPixelType;
  typedef typename TOutputImage::PixelType                  OutputPixelType;

  /** Method for creation through the object factory. */
  itkNewMacro(Self);

  /** Run-time type information (and related methods). */
  itkTypeMacro(ImageFilter, ImageToImageFilter);
```

Filter Impl - 3

Look at ITK Macros :

```
  itkSetMacro(Low, InputPixelType);
  itkGetMacro(Low, InputPixelType);
  itkSetMacro(High, InputPixelType);
  itkGetMacro(High, InputPixelType);

protected:
  MyThresholdFilter(){}
  ~MyThresholdFilter(){}
```

Filter Impl - 4

The main method :

```
  /** Does the real work. */
  virtual void GenerateData()
  {
    TInputImage  *inputImage  = static_cast< TInputImage  * >(this->ProcessObject::GetInput(
    TOutputImage *outputImage = static_cast< TOutputImage * >(this->ProcessObject::GetOutput

    ImageRegionConstIterator<TInputImage> inputIterator = ImageRegionConstIterator<TInputIma
    ImageRegionIterator<TOutputImage> outputIterator = ImageRegionIterator<TOutputImage>(out


    for (inputIterator.GoToBegin(),
         outputIterator.GoToBegin();
         !inputIterator.IsAtEnd() && !outputIterator.IsAtEnd();
         ++inputIterator,
         ++outputIterator)
    {
      if (*inputIterator >= m_Low && *inputIterator <= m_High)
      {
        *outputIterator = 1;
      }
      else
      {
        *outputIterator = 0;
      }
    }
  }

private:
  MyThresholdFilter(const Self &); //purposely not implemented
  void operator=(const Self &);  //purposely not implemented
```

```
  InputPixelType m_Low;
  InputPixelType m_High;
};
} // end namespace

int main(int argc, char** argv)
{
  // Not providing a real example,
  // as I dont know how to read/write images within the
  // dexy framework.
  return 0;
}
```

Iterators

- ITK provides many iterators
- Generic Programming means:
  - Suitable for n-dimensions
  - Suitable for all types of data
- Also, different image access concepts
  - Region of Interest
  - Random subsampling
  - No change in code
- So iterators enable you to traverse image and encapsulate the traversal mechanism in an iterator

- Similar concept to STL `.begin()`, `.end()`
- See ITK Software Guide

Private Constructors?

If you look at an ITK filter, you may notice for example

```
protected:
  AddImageFilter() {}
  virtual ~AddImageFilter() {}

private:
  AddImageFilter(const Self &);
  void operator=(const Self &);
```

- Copy constructor and copy assignment are private and not implemented
- Constructor and Destructor private. So how do you use?

Static New Method

You will then see

```
/** Method for creation through the object factory. */
itkNewMacro(Self);
```

which if you hunt for long enough, you find this snippet

```
#define itkSimpleNewMacro(x)
  static Pointer New(void)
    {
    Pointer smartPtr = ::itk::ObjectFactory< x >::Create();
    if ( smartPtr.GetPointer() == ITK_NULLPTR )
      {
      smartPtr = new x;
      }
    return smartPtr;
    }
```

So, either this `ObjectFactory` creates it, or a standard `new` call.

ObjectFactory::Create

In `itk::ObjectFactory` we ask factory to CreateInstance using a `char*`

```
static typename T::Pointer Create()
{
  LightObject::Pointer ret = CreateInstance( typeid( T ).name() );
  return dynamic_cast< T * >( ret.GetPointer() );
}
```

`CreateInstance` works with either a base class name, or a class name to return either a specific class, or a family of classes derived from a common base class.

Why Object Factories?

- Rather than create objects directly
- Ask a class (ObjectFactory) to do it
- This class contain complex logic, not just a new operator
- So, we can
    - dynamically load libraries from ITK_AUTOLOAD_PATH at runtime

  - Have a list/map of current classes, and provide overrides
  - i.e swap in a GPU version instead of CPU
- More dynamic variant of FactoryMethod, AbstractFactory (See GoF)

File IO Example

In `itkImageFileReader.hxx`

```
std::list< LightObject::Pointer > allobjects =
  ObjectFactoryBase::CreateAllInstance("itkImageIOBase");
```

- We ask the factory for every class that is a sub-class of itkImageIOBase.
- Then we can ask each ImageIOBase sub-class if it can read a specific format.
- First one to reply true reads the image.
- In general case, ask ObjectFactoryBase for any class.

Object Factory List of Factories

In class ObjectFactoryBase

```
class  ObjectFactoryBase:public Object
{
public:
  static std::list< ObjectFactoryBase * > GetRegisteredFactories();
```

This class maintains a static vector of ObjectFactoryBase. These are added programmatically, via static initialisation or dynamically via the ITK_AUTO_LOAD_PATH.

PNG IO Factory

- Given `itkPNGImageIO.h/cxx` can read PNG images
- We see in `itkPNGImageIOFactory.cxx`

```
PNGImageIOFactory::PNGImageIOFactory()
{
  this->RegisterOverride( "itkImageIOBase",
                          "itkPNGImageIO",
                          "PNG Image IO",
                          1,
                          CreateObjectFunction< PNGImageIO >::New() );
}
```

So, PNG factory says it implements a type of itkImageIOBase, will return an itkPNGImageIO, and instantiates a function object that calls the right constructor.

ObjectFactory Summary

- ObjectFactory defines a static vector of ObjectFactory
- ObjectFactory objects loaded:
  - Directly named in code at compile time
  - Via static initialisers when a dynamic library is loaded
  - Or from ITK_AUTOLOAD_PATH
- ObjectFactory returns one/all classes that implement a given class
- Static New method now asks factory for a class.
- So, you can override any ITK class.
- Why is above example not an infinite loop?

ITK Summary

- Pipeline architecture for most filters
- Also includes a registration framework (see ITK Software Guide)
- Smart Pointers - reference counting, automatic deletion
- Static New method with ObjectFactory to enable overriding any class at runtime
- Dynamic loading via ITK_AUTOLOAD_PATH
- Pipeline architecture - easy to prototype, once you know C++
- Write your own filter, unit test, generalise to n-dimension, of n-vectors.
- Easy to extend to multi-threading

Summary

Learning Objectives

- Use well written libraries
- Understand enough C++ for some common C++ libraries

Further Reading

Please refer to the following:

- Short Eigen Tutorial
- Longer Eigen Tutorial
- Boost Tutorials for each library
- ITK Software Guide
- Simple ITK: Template free, wrapper, python, paper

Chapter 5

HPC Concepts

High Performance Computing Overview

Background Reading

- This section is based on background reading outside the classroom
- This will save time in the classroom for practical work
- But you do need to know this content
- Read:
  - SUNY HPC notes
  - Herb Sutter's "Welcome to the Jungle"
  - Some background history on Wikipedia
  - [Blaise Barney's overview of parallel computing][https://computing.llnl.gov/tutorials/parallel_comp/]

Essential Reading

- For the exam you will need:
  - Amdahl's law
  - Flynn's Taxonomy
- For tutorial's and practical work you will need:
  - Use of unix shell
  - Submitting jobs on a cluster
  - See RITS HPC Training
  - We'll recap this now

Aim

For the remainder of the course, we need to develop

- Skills to run jobs on a cluster, e.g. Legion.
- A locally installed development environment, so you can develop
- Familiarity with new technologies, OpenMP, MPI, Accelerators, Cloud, so you can make a reasoned choice

Chapter 6

Shared memory parallelism

Shared Memory Parallelism

OpenMP

- Shared memory only parallelization
- Useful for parallelization on a single cluster node
- MPI next week for inter-node parallelization
- Can write hybrid code with both OpenMP and MPI

About OpenMP

- Extensions of existing programming languages
- Standardized by international committee
- Support for Fortran, C and C++
- C/C++ uses the same syntax
- Fortran is slightly different

How it works

- Thread based parallelization
- A master thread starts executing the code.
- Sections of the code is marked as parallel
    - A set of threads are forked and used together with the master thread
    - When the parallel block ends the threads are killed or put to sleep

Typical use cases

- A loop with independent iterations
- Hopefully a significant part of the execution time
- More complicated if an iterations have dependencies

OpenMP

OpenMP basic syntax

- Annotate code with `#pragma omp ...`
  - This instruct the compiler in how to parallize the code
  - `#pragma`s are a instructions to the compiler
  - Not part of the language
  - i.e. `#pragma once` alternative to include guards
  - Compiler will usually ignore pragmas that it doesn't understand
  - All OpenMP pragmas start with `#pragma omp`
- OpenMP must typically be activated when compiling code

OpenMP library

- OpenMP library:
  - It provides utility functions.
  - `omp_get_num_threads()` ...
  - Use with `#include <omp.h>`

Compiler support

OpenMP is supported by most compilers, except LLVM/Clang(++)

- OpenMP must typically be activated with a command line flags at compile time. Different for different compilers. Examples:
  - Intel, Linux, Mac `-openmp`
  - Intel, Windows `/Qopenmp`
  - GCC/G++, `-fopenmp`

A fork of clang with OpenMP exists. It might make it into the mainline eventually.

Hello world

```
#include <iostream>
#include <omp.h>

int main(int argc, char ** argv)
{
    #pragma omp parallel
    {
        int threadnum = 0;
        int numthreads = 0;
        threadnum = omp_get_thread_num();
        numthreads = omp_get_num_threads();
        std::cout << "Hello World, I am " << threadnum
            << " of " << numthreads << std::endl;
    }
}
```

- `#pragma omp parallel` marks a block is to be run in parallel
- In this case all threads do the same
- No real work sharing

Issues with this example

- `std::cout` is not thread safe. Output from different threads may be mixed
  - Try running the code
  - Mixed output?
- All threads call `omp_get_num_threds()` with the same result
  - Might be wasteful if this was a slow function
  - Everybody stores a copy of numthreads
  - Waste of memory

Slightly improved hello world

```
#include <iostream>
#ifdef _OPENMP
#include <omp.h>
#endif

int main(int argc, char ** argv)
{
    int threadnum = 0;
```

```
    int numthreads = 0;
    #pragma omp parallel shared(numthreads), private(threadnum)
    {
        #ifdef _OPENMP
            threadnum = omp_get_thread_num();
            #pragma omp single
            {
                numthreads = omp_get_num_threads();
            }
        #endif
        #pragma omp critical
        {
            std::cout << "Hello World, I am " << threadnum <<
                " of " << numthreads << std::endl;
        }
    }
}
```

Improvements:

- Use `#pragma omp critical` to only allow one thread to write at a time
  - Comes with a performance penalty since only one thread is running this code at a time
- Use Preprocessor `#ifdef _OPENMP` to only include code if OpenMP is enabled
  - Code works both with and without OpenMP
- Variables defined outside parallel regions
  - Must be careful to tell OpenMP how to handle them
  - `shared`, `private`, `first private`
  - More about this later
- `#pragma omp single`
  - Only one thread calls `get_num_threds()`

Running OpenMP code for the course

If you have a multicore computer with GCC or other suitable compiler you can run it locally.

Otherwise you can use GCC on aristotle

- `ssh username@aristotle.rc.ucl.ac.uk`

- `module load GCC/4.7.2`
- `g++ -fopenmp -O3 mycode.cc`

References

- OpenMP homepage
- OpenMP cheat sheet
- OpenMP specifications

Parallelizing loops with OpenMP

Simple example

Integrate:

$\int_0^1 \frac{4}{1+x^2} \mathrm{d}x = \pi$

```
#include <iostream>

int main(int argc, char ** argv)
{
    double pi,sum,x;
    const int N = 10000000;
    const double w = 1.0/N;

    pi = 0.0;
    sum = 0.0;
    #pragma omp parallel private(x), firstprivate(sum), shared(pi)
    {
        #pragma omp for
        for (int i = 0; i < N; ++i)
        {
            x = w*(i-0.5);
            sum = sum + 4.0/(1.0 + x*x);
        }
        #pragma omp critical
        {
            pi = pi + w*sum;
        }
    }
    std::cout << "Result is " << pi << std::endl;
}
```

Variable scope

- Private: Each thread has it's own copy
- Shared: Only one shared variable
- Firstprivate: Private variable but initialized with serial value

Details of example

- Important that `x` and `sum` are private
  - Try making them shared and see what happens
- Note that the default is shared
  - Can be controlled with the default clause
  - `default(none)` is safer
  - "Explicit is better that implicit"
- We use a critical region to add safely without a race condition

Reduction

- Aggregating a result from multiple threads with a single mathematical operation
- Is a very common pattern
- OpenMP has build in support for doing this
- Simplifies the code and avoids the explicit critical region
- Easier to write and may perform better

Reduction example

```
#include <iostream>

int main(int argc, char ** argv)
{
    double pi,sum,x;
    const int N = 10000000;
    const double w = 1.0/N;

    pi = 0.0;
    sum = 0.0;

    #pragma omp parallel private(x), reduction(+:sum)
    {
        #pragma omp for
```

```
        for (int i = 0; i < N; ++i)
        {
            x = w*(i-0.5);
            sum = sum + 4.0/(1.0 + x*x);
        }
    }
    pi = w*sum;
    std::cout << "Result is " << pi << std::endl;
}
```

Races, locks and critical regions

Introduction

In the best of worlds our calculations can be done independently. However, even in our simplest examples we saw issues.

- `std::cout` is not thread safe. Garbage mixed output
- Needs to use `critical` to merge output
- Real world examples may be more complicated
- Incorrectly shared variable leads to random and typically wrong results

Race condition

When the result of a calculation depends on the timing between threads.

- Example: threads writing to same variable
- Can be hard to detect
- May only happen in rare cases
- May only happen on specific platforms
- Or depend on system load from other applications

Barriers and synchronisation

Typically it is necessary to synchronize threads. Make sure that all threads are done with a piece of work before moving on. Barriers synchronizes threads.

- Parallel regions such as `omp for` have an implicit barrier at the end
    - Threads wait for the last to finish before moving on
    - May waste significant amount of time

  - We will return to look at load balancing later
  - Sometime there is no need to wait
  - Disable implicit barrier with `nowait`
- Sometimes you need a barrier where there is no implicit barrier
  - `#pragma omp barrier` inserts a barrier
  - Don't overuse this. Performance drop

Protecting code and variables

- `#pragma omp critical`
  - Only one task can execute at a time
  - Protect non thread-safe code
- `#pragma omp single`
  - Only one tread executes this block
  - The first thread that arrives will execute the code
- `#pragma omp master`
  - Similar to singe but uses the master thread
- `#pragma omp atomic`
  - Protect a variable by changing it in one step.

Mutex locks

Sometimes the critical regions are not flexible enough to implement your algorithm.

Examples:

- Need to prevent two different pieces of code from running at the same time.
- Need to lock only a fraction of a large array.

OpenMP locks

OpenMP locks is a general way to manage resources in threads.

- A thread tries to set the lock.
- If the lock is not held by any other thread it is successful and free to carry on.
- If not it will wait until the lock becomes unset.
- Important to remember to unset the lock when done.
- Might otherwise result in a deadlock. Program hangs.

Example

Replace the critical region with a lock. In this case there is no real gain from using a lock.

```
#include <iostream>
#include <omp.h>

int main(int argc, char ** argv)
{
    double pi,sum,x;
    const int N = 10000000;
    const double w = 1.0/N;
    omp_lock_t writelock;
    pi = 0.0;
    sum = 0.0;
    #pragma omp parallel private(x), firstprivate(sum), shared(pi)
    {
        #pragma omp for
        for (int i = 0; i < N; ++i)
        {
            x = w*(i-0.5);
            sum = sum + 4.0/(1.0 + x*x);
        }
        omp_set_lock(&writelock);
        pi = pi + w*sum;
        omp_unset_lock(&writelock);
    }
    omp_destroy_lock(&writelock);
    std::cout << "Result is " << pi << std::endl;
}
```

Multiple locks

Sometimes it is useful to lock multiple resources with different locks.

- Use multiple locks protecting different resources
- Can result in deadlocks if two threads needs both needs the same locks
- One thread holds one lock and the other one holds the other
- Both are waiting for a lock to be free

Notes

OpenMP implements two types of locks. We have only considered simple locks. Consult the OpenMP specifications for nested locks.

OpenMP Tasks

Introduction

- Not all problems are easily expressed as for loops.
- The task construction creates a number of tasks
- The tasks are added to a queue
- Threads take a task from the queue

Example

Calculate Fibonacci numbers by recursion.

- Only as an example:
  - Hard to get any performance improvement. Usually slower that serial code
  - Inefficient algorithm in any case. Why?
  - Consider limiting the number of tasks. Why?
- Use taskwait to ensure results are done before adding their results together

Code

```
#include <iostream>
#ifdef _OPENMP
#include <omp.h>
#endif

int fib(int n)
{
    if (n < 2)
        return n;
    int x;
    int y;
    const int tune = 40;
    #pragma omp task firstprivate(n) shared(x)
```

```
    {
        x = fib(n-1);
    }
    #pragma omp task firstprivate(n) shared(y)
    {
       y = fib(n-2);
    }
    #pragma omp taskwait

    return x + y;
}
```

Main function

```
int main(int argc, char ** argv)
{
    #ifdef _OPENMP
    omp_set_dynamic(0);
    #endif
    const int num = 20;
    int a;
    #pragma omp parallel shared(a)
    {
        #pragma omp single nowait
        {
        a = fib(num);
       }
    }
    std::cout << "fib " << num << " is " << a << std::endl;
}
```

Note only one thread initially creates tasks. Tasks are still running in parallel.

Advanced usage

- Task dependency:
    - Depends on child tasks. `#taskwait`
    - Real cases may be more complicated
    - May need to explicitly set dependency
    - `#pragma omp task depends(in/out/inout:variable)`
    - See OpenMP docs for details
- `taskyield` Allows a task to be suspended in favour of a different task:

- Could be useful together with locks

Controlling task generation

- `if(expr) expr==false` create an undeferred task
  - Suspend the present task and execute the new task immediately on the same tread
- `final(expr) expr==true` This is the final task
  - All child tasks are included in the present task
- `mergeable`
  - Included and undeferred tasks may be merged into the parent task

May useful to avoid creating to many small tasks. I.e. in our Fibonacci example.

Scheduling and Load Balancing

Number of threads

The number of threads executing an OpenMP code is determined by the environmental variable `OMP_NUM_THREADS`.

Normally `OMP_NUM_THREADS` should be equal to the number of CPU cores

Load balancing

Consider our earlier example of a for loop. 10000000 iterations split on 4 cores

Two obvious strategies:

- Split in 4 chunks:
  - 2500000 iterations for each core
  - Minimal overhead for managing threads
  - Probably a good solution if the cost is independent of `i`
  - But what if the cost depended on `i`
  - One tread might be slower than the rest
- Give each thread one iteration at a time
  - No idling thread
  - But huge overhead

The best solution is probably somewhere in between.

OpenMP strategies

OpenMP offers a number of different strategies for load balancing set by the following key words. The default is static with one chunk per thread.

- `static`: Iterations are divided into chunks of size `chunk_size` and assigned to threads in round-robin order
- `dynamic`: Each thread executes a chunk of iterations then requests another chunk until none remain
- `guided`: Like dynamic but the chunk size depends on the number of remaining iterations
- `auto`: The decision regarding scheduling is delegated to the compiler and/or runtime system
- `runtime`: The schedule and chunk size are controlled by runtime variables

Which strategy to use

It is hard to give general advice on the strategy to use. Depends on the problem and platform. Typically needs benchmarking and experimentation.

- If there is little variation in the runtime of iteration static with a large chunk size minimizes overhead
- In other cases it might make sense to reduce the chunk size or use dynamic or guided
- Note that both dynamic and guided comes with additional overhead to schedule the distribution of work

Alternatives to OpenMP

Overview

- OpenACC:
  - Similar to OpenMP but intended for accelerators. Lecture 9
- MPI:
  - For distributed memory systems. Next lecture
- POSIX and Windows threads. Not portable across operation systems
- C++ 11 threads
- Intel Threading Building Blocks C++ only template library
  - Somewhat more complicated. Requires good understanding of templated code
- Intel Cilk Plus C and C++, Intel and GCC >= 4.9 only

C++11

Simple example:

```
#include <thread>
#include <iostream>

void f()
{
    std::cout << "Hello" << std::endl;
};

void g()
{
    std::cout << "world" << std::endl;
};


int main(int argc, char ** argv)
{
    std::thread t1 {f};
    std::thread t2 {g};

    t1.join();
    t2.join();
}
```

Details

- Same problem as first OpenMP example. `std::cout` is not thread safe
    - Use mutex and locks
- Queues
- Futures and promise
- packed_task

Likely more suited for multi threaded desktop applications than scientific software.

Cilk Plus

```
#include <iostream>
#include <time.h>
```

```
#include <cilk/cilk.h>
#include <cilk/cilk_api.h>

int fib(int n)
{
    if (n < 2)
        return n;
    int x = cilk_spawn fib(n-1);
    int y = fib(n-2);
    cilk_sync;
    return x + y;
}

int main(int argc, char ** argv)
{

    const int n = 35;
    if (argc > 1)
    {
        // Set the number of workers to be used
        __cilkrts_set_param("nworkers", argv[1]);
    }

    int a = fib(n);
    std::cout << "fib(" << n << ") is " << a << std::endl;
}
```

Further Reading

Tutorials

Any additional tutorials can be added here:

- Blaise Barney, Lawrence Livermore National Laboratory

Chapter 7

Distributed memory parallelism

Distributed Memory Parallelism

The basic idea

- many processes, each with their own data

- each process is independent
- processes can send messages to one another

MPI in practice

Specification and implementation

- in practice, we use MPI, the Message Passing Interface
- MPI is a *specification* for a *library*
- It is implemented by separate vendors/open-source projects
  - OpenMPI
  - mpich

- It is a C library with many many bindings:
  - Fortran (part of official MPI specification)
  - Python: boost, mpi4py
  - R: Rmpi
  - c++: boost

Programming and running

- an MPI program is executed with `mpiexec -n N [options] nameOfProgram [args]`
- MPI programs call methods from the mpi library

```
int MPI_Bcast(void *buffer, int count, MPI_Datatype datatype, int root,
              MPI_Comm comm)
```

- vendors provide wrappers (mpiCC, mpic++) around compilers. Wrappers point to header file location and link to right libraries. MPI program can be (easily) compiled by substituting `(g++|icc) -> mpiCC`

Hello, world!: hello.cc

```
#include <mpi.h>
#include <iostream>

int main(int argc, char * argv[]) {
    /// Must be first call
    MPI_Init (&argc, &argv);
    /// Now MPI calls possible

    /// Size of communicator and process rank
    int rank, size;
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
    MPI_Comm_size (MPI_COMM_WORLD, &size);

    std::cout << "Processor " << rank << " of " << size << " says hello\n";

    /// Must be last MPI call
    MPI_Finalize();
    /// No more MPI calls from here
    return 0;
}
```

Hello, world!: CMakeLists.txt

```
cmake_minimum_required(VERSION 2.8)

find_package(MPI REQUIRED)

include_directories(${MPI_C_INCLUDE_PATH})
set(CMAKE_CXX_FLAGS "${CMAKE_CXX_FLAGS} ${MPI_C_COMPILE_FLAGS}")

add_executable(hello hello.cc)
target_link_libraries(hello ${MPI_C_LIBRARIES} ${MPI_CXX_LIBRARIES})
```

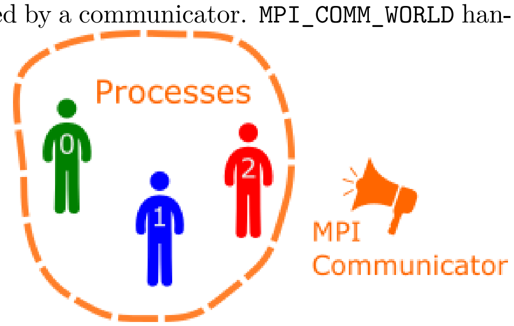
Hello, world!: compiling and running

On aristotle.rc.ucl.ac.uk:

- load modules: `module load GCC/4.7.2 OpenMPI/1.6.4-GCC-4.7.2` `module load cmake/2.8.10.2`
- create files "hello.cc" and "CMakeLists.txt" in some directory
- create build directory `mkdir build && cd build`
- run cmake and make `cmake .. && make`
- run the code `mpiexec -n 4 hello`

Hello, world! dissected

- MPI calls *must* appear beween `MPI_Init` and `MPI_Finalize`
- Groups of processes are handled by a communicator. `MPI_COMM_WORLD` han-



dles the group of all processes.
- Size of group and rank (order) of process in group
- By *convention*, process of rank 0 is *special* and called *root*

MPI with CATCH

Running MPI unit-tests requires MPI_Init and MPI_Failure before and after the test framework (*not* inside the tests).

```
#include <mpi.h>
// Next line tells CATCH we will use our own main function
#define CATCH_CONFIG_RUNNER
#include "catch.hpp"

TEST_CASE("Just test I exist") {
    int rank, size;
    MPI_Comm_rank (MPI_COMM_WORLD, &rank);
    MPI_Comm_size (MPI_COMM_WORLD, &size);
    CHECK(size > 0); CHECK(rank >= 0);
}

int main(int argc, char * argv[]) {
    MPI_Init (&argc, &argv);
    int result = Catch::Session().run(argc, argv);
    MPI_Finalize();
    return result;
}
```

Point to point communication

Many point-2-point communication schemes

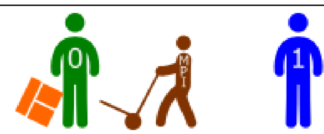
Can you think of two behaviours for message passing?

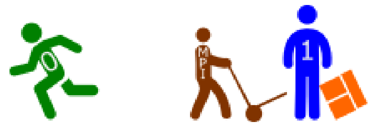
- Process 0 can (i) give message and then either (ii) leave or (iii) wait for acknowledgements
- Process 1 can (i) receive message
- MPI can (i) receive message, (ii) deliver message, (iii) deliver acknowledgments

Blocking synchronous send

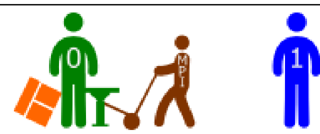
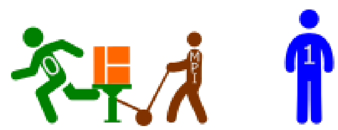
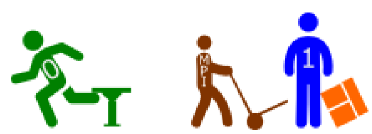
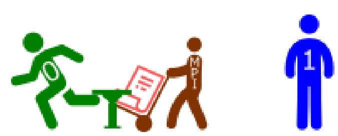
Stage	Figure
a. 0, 1, and MPI stand ready:	
b. message dropped off by 0:	
c. transit:	
d. message received by 1	
e. receipt received by 0	

Blocking send

Stage	Figure
a. 0, 1, and MPI stand ready:	
b. message dropped off by 0:	
c. transit, 0 leaves	

Stage	Figure
d. message received by 1	

Non-blocking send

Stage	Figure
a. 0, 1, and MPI stand ready:	
b. 0 leaves message in safebox	
c. transit	
d. message received by 1	
e. receipt placed in safebox	

Blocking synchronous send

```
int MPI_Ssend(const void *buf, int count, MPI_Datatype datatype, int dest, int tag,
              MPI_Comm comm)
```

Parameter	Meaning
buf	Pointer to buffer. Always `void` because practical C is not type safe.

Parameter	Meaning
count	Size of the buffer. I.e. length of the message to send, in units of the specified datatype (not byte
datatype	Encodes type of the buffer. `MPI_INT` for integers, `MPI_CHAR` for characters. Lots of others.
dest	Rank of the *receiving* process
tag	A tag for message book-keeping
comm	The communicator – usually just `MPI_COMM_WORLD`
return	An error tag. Equals `MPI_SUCCESS` on success.

Blocking receive

```
int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source, int tag,
             MPI_Comm comm, MPI_Status *status)
```

Good for both synchronous and asynchonous communication

Parameter	Meaning
buf	Pointer to receiving *pre-allocated* buffer
count	Size of the buffer. I.e. maximum length of the message to receive. See `MPI_Get_count`
datatype	Informs on the type of the buffer
source	Rank of the *sending* process
tag	A tag for message book-keeping
status	‘MPI_STATUS_IGNORE`for now. See`MPI_Get_count“.
comm	The communicator
return	Error tag

Example: Blocking synchronous example

Inside a new section in the test framework:

```
std::string const peace = "I come in peace!";
if(rank == 0) {
   int const error = MPI_Ssend(
     (void*) peace.c_str(), peace.size() + 1, MPI_CHAR, 1, 42, MPI_COMM_WORLD);
```

```
        // Here, we guarantee that Rank 1 has received the message.
        REQUIRE(error ==  MPI_SUCCESS);
    }
    if(rank == 1) {
        char buffer[256];
        int const error = MPI_Recv(
          buffer, 256, MPI_CHAR, 0, 42, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
        REQUIRE(error ==  MPI_SUCCESS);
        CHECK(std::string(buffer) == peace);
    }
```

Common bug: Set both sender and receiver to 0. What happens?

Example: Do you know your C vs C++ strings?

Why the `+1`?

```
int const error = MPI_Ssend(
  (void*) peace.c_str(), peace.size() + 1, MPI_CHAR, 1, 42, MPI_COMM_WORLD);
```

. . .

Because C and C++ `char const*` strings are null-terminated to indicate the string is finished, which adds an extra character. However, `std::string` abstracts it away. And so its length does *not* include the null-termination.

Example: Causing a dead-lock

Watch out for order of send and receive!

Bad:

```
if(rank == 0) {
   MPI_Ssend (sendbuf, count, MPI_INT, 1, tag, comm);
   MPI_Recv (recvbuf, count, MPI_INT, 1, tag, comm, &status);
} else {
   MPI_Ssend (sendbuf, count, MPI_INT, 0, tag, comm);
   MPI_Recv (recvbuf, count, MPI_INT, 0, tag, comm, &status);
}
```

Good:

```
if(rank == 0) {
   MPI_Ssend (sendbuf, count, MPI_INT, 1, tag, comm);
   MPI_Recv (recvbuf, count, MPI_INT, 1, tag, comm, &status);
} else {
   MPI_Recv (recvbuf, count, MPI_INT, 0, tag, comm, &status);
   MPI_Ssend (sendbuf, count, MPI_INT, 0, tag, comm);
}
```

Send vs SSend

Why would we use Send instead of SSend?

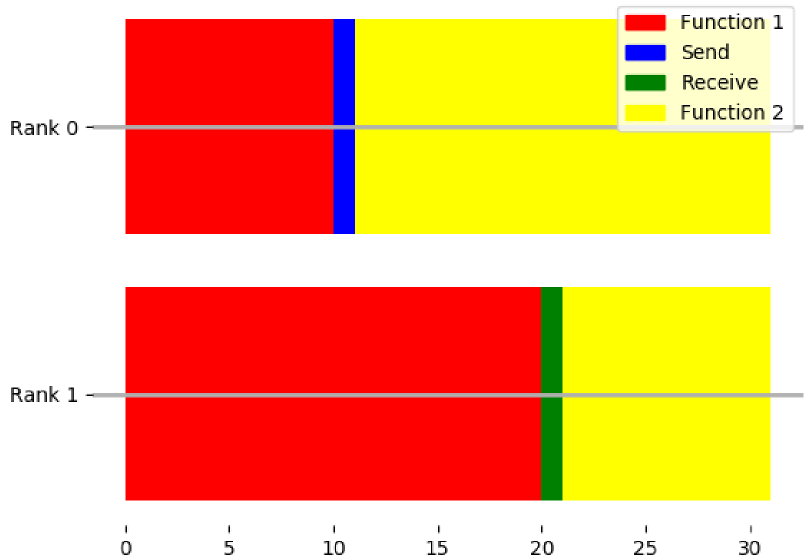
```
std::string peace = "I come in peace!";
if(rank == 0) {
   int const error = MPI_Send(
     (void*) peace.c_str(), peace.size() + 1, MPI_CHAR, 1, 42, MPI_COMM_WORLD);
   // We do not guarantee that Rank 1 has received the message yet
   // But nor do we necessarily know it hasn't.
   // But we are definitely allowed to change the string, as MPI promises
   // it has been buffered
   peace = "Shoot to kill!"; // Safe to reuse the send buffer.
   REQUIRE(error ==  MPI_SUCCESS);
}
if(rank == 1) {
    char buffer[256];
    int const error = MPI_Recv(
      buffer, 256, MPI_CHAR, 0, 42, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
    REQUIRE(error ==  MPI_SUCCESS);
    CHECK(std::string(buffer) == peace);
}
```

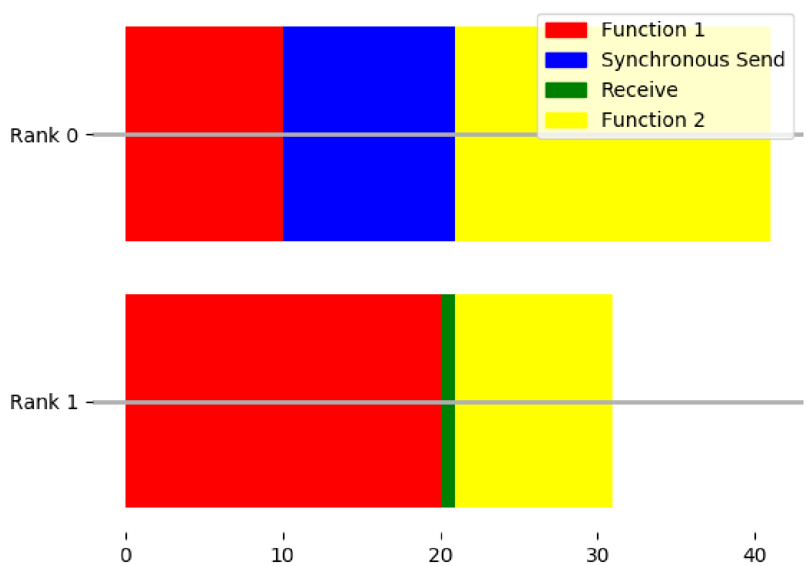
Both guarantee the buffer is safe to reuse. Send makes no guarantee as to whether it returns early or not. But *SSend* forces a *synchronisation point*: the codes reach the matching places, with all processes waiting until all reach that point.

It may come out slightly faster to use Send, since having a **synchronisation point** when you don't need one can slow things down: Suppose (A) runs slightly faster, then (B) does; at the end, they've both been running fully efficiently.

Wth a synchronisation point in between, you'll have wasted time:

This is only important when there is noise or variability in the execution time on different processes, but this is often the case.


Function 1
Send
Receive
Function 2
Rank 0
Rank 1
0
5
10
15
20
25
30


Function 1
Synchronous Send
Receive
Function 2
Rank 0
Rank 1
0
10
20
30
40

So unnecessary synchronisation points are bad. The MPI Implementation may choose to buffer, or synchronise in Send; you're letting MPI guess.

However, if you want to fine tune this to get the best performance, you should use ISend.

Non-blocking: ISend/IRecv

With ISend, we indicate when we want the message to set off.

We receive a handle to the message, of type `MPI_Request*` which we can use to require it has been received, or check.

This produces more complicated code, but you can write code which **overlaps calculation with communication**: the message is travelling, while you get on with something else. We'll see a practical example of using this next lecture.

```
std::string peace = "I come in peace!";
if(rank == 0) {
  MPI_Request request;
   int error = MPI_Isend(
     (void*) peace.c_str(), peace.size() + 1, MPI_CHAR, 1, 42,
     MPI_COMM_WORLD, &request);
   // We do not guarantee that Rank 1 has received the message yet
   // We can carry on, and ANY WORK WE DO NOW WILL OVERLAP WITH THE
   // COMMUNICATION
   // BUT, we can't safely change the string.
   REQUIRE(error ==  MPI_SUCCESS);
   // Do some expensive work here
   for (int i=0; i<1000; i++) {}; // BUSYNESS FOR EXAMPLE
   MPI_Status status;
   error = MPI_Wait(&request, &status);
   REQUIRE(error ==  MPI_SUCCESS);
   // Here, we run code that requires the message to have been
   // successfully sent.
}
if(rank == 1) {
    char buffer[256];
    int const error = MPI_Recv(
      buffer, 256, MPI_CHAR, 0, 42, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
    REQUIRE(error ==  MPI_SUCCESS);
    CHECK(std::string(buffer) == peace);
}
```

```
int MPI_Isend(const void *buf, int count, MPI_Datatype datatype, int dest, int tag,
              MPI_Comm comm, MPI_Request *request)
```

Pass the parcel: SendRecv

Consider a group of N processes in a ring: each has a value, and wants to "pass the parcel" to the left. How would you achieve this with SSend and Receive?

```
int message = rank*rank;
int received = -7;

// Define the ring
int left = rank-1;
int right = rank+1;
if (rank==0) {
  left = size-1;
}
if (rank == size-1){
  right = 0;
}
```

With synchronous calls each process can only either be sending or receiving. So the even processes need to send, while the odd ones receive, then vice-versa. This is clearly inefficient.

```
if (rank%2 == 0) {
  int error = MPI_Ssend(
    &message, 1, MPI_INT, left, rank, MPI_COMM_WORLD);

  error = MPI_Recv(
    &received, 1, MPI_INT, right, right, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
}
if (rank%2 == 1) {

  int error = MPI_Recv(
    &received, 1, MPI_INT, right, right, MPI_COMM_WORLD, MPI_STATUS_IGNORE);

  error = MPI_Ssend(
    &message, 1, MPI_INT, left, rank, MPI_COMM_WORLD);
}
REQUIRE( received == right*right );
```

With ISend/IRecv, this can be achieved in one go: each process posts its send, then posts its receive, then waits for completion.

```
MPI_Request request;
// Everyone sets up their messages to send
int error = MPI_Isend(
  &message, 1, MPI_INT, left, rank, MPI_COMM_WORLD, &request);

// Recv acts as our sync-barrier
error = MPI_Recv(
  &received, 1, MPI_INT, right, right, MPI_COMM_WORLD, MPI_STATUS_IGNORE);

// But let's check our send completed:
error = MPI_Wait(&request, MPI_STATUS_IGNORE);
REQUIRE(error ==  MPI_SUCCESS);

REQUIRE( received == right*right );
```

However, this is such a common pattern, that there is a separate MPI call to make this easier:

```
int MPI_Sendrecv(void *sendbuf, int scount, MPI_Datatype stype, int dest, int stag,
                 void *recvbuf, int rcount, MPI_Datatype rtype, int source, int rtag,
                 MPI_Comm comm, MPI_Status *status)
```

Each argument is duplicated for the send and receive payloads.

Classroom exercise: implement ring-send using Sendrecv.

Al(most all) point to point

Sending messages:

name	Blocking	forces synchronisation point	Buffer-safe
MPI_Ssend	yes	yes	yes
MPI_Send	maybe	no	yes
MPI_Isend	no	no	no

Receiving messages:

name	blocking
MPI_Recv	yes

name	blocking
MPI_Irecv	no

Collective Communication

Many possible communication schemes

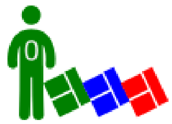
Think of two possible forms of *collective* communications:

- give a beginning state
- give an end state

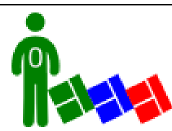
Broadcast: one to many

State	Figure		
data in 0, no data in 1, 2			
data from 0 sent to 0, 1			

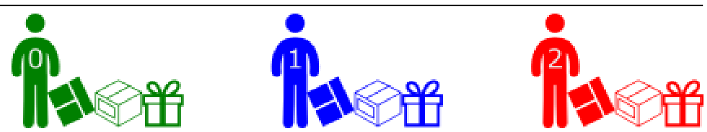
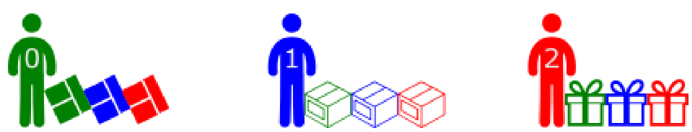
Gather: many to one

State	Figure
data in 0, 1, 2	
data from 1, 2 sent to 0	

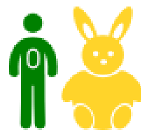
Scatter: one to many

State	Figure
data in 0	
data from 0 in 0, 1, 2	

All to All: many to many

State	Figure
data in 0, 1, 2	
from each to each	

Reduce operation

State	Figure		
data in 0, 1, 2			
Baby Bunny!			

Wherefrom the baby bunny?

. . .

Sum, difference, or any other *binary* operator:

Collective operation API

Group synchronisation:

```
int MPI_Barrier(MPI_Comm comm);
```

Broadcasting:

```
int MPI_Bcast(void *buffer, int count, MPI_Datatype datatype, int root,
    MPI_Comm comm)
```

Parameter	Content
buf	Pointer to sending/receiving buffer
count	Size of the buffer/message
datatype	Informs on the type of the buffer
root	Sending processor
comm	The communicator!
return	Error tag

Example of collective operation (1)

Insert into a new CATCH section the following commands

```
std::string const peace = "I come in peace!";
std::string message = "";
int error;
if(rank == 0) {
    message = peace;
    error = MPI_Bcast(
       (void*) peace.c_str(), peace.size() + 1, MPI_CHAR, 0, MPI_COMM_WORLD);
} else {
    char buffer[256];
    error = MPI_Bcast(buffer, 256, MPI_CHAR, 0, MPI_COMM_WORLD);
    message = std::string(buffer);
}
```

Example of collective operations (2)

And then insert the following right after it

```
for(int i(0); i < size; ++i) {
    if(rank == i) {
      INFO("Current rank is " << rank);
      REQUIRE(error == MPI_SUCCESS);
      CHECK(message == peace);
    }
    MPI_Barrier(MPI_COMM_WORLD);
}
```

Causing deadlocks

Explain why the following two codes fail.

1. Replace the loop in the last fragment with:

```
for(int i(1); i < size; ++i) ...
```

2. Refactor and put everything inside the loop

```cpp
std::string const peace = "I come in peace!";
std::string message;
for(int i(0); i < size; ++i) {
    if(i == 0 and rank == 0) { /* broadcast */ }
    else if(rank == i) { /* broadcast */ }
    if(rank == i) { /* testing bit */ }
    MPI_Barrier(MPI_COMM_WORLD);
}
```

NOTE: a loop with a condition for i == 0 is a common anti-pattern (eg bad)

All to all operation

```cpp
int MPI_Scatter(const void *sendbuf, int sendcount, MPI_Datatype sendtype,
                void *recvbuf, int recvcount, MPI_Datatype recvtype, int root,
                MPI_Comm comm)
```

Parameter	Content
sendbuf	Pointer to sending buffer (only significant at root)
sendcount	Size of a *single* message
datatype	Type of the buffer
recvbuf	Pointer to receiving buffers (also at root)
recvcount	Size of the receiving buffer
recvtype	Informs on the type of the receiving buffer

Exercise: Have the root scatter "This….." "message.." "is.split." to 3 processors (including it self).

Splitting the communicators

Groups of processes can be split according to *color*:

```cpp
int MPI_Comm_split(MPI_Comm comm, int color, int key, MPI_Comm *newcomm)
```

Parameter	Content
comm	Communicator that contains all the processes to be split

Parameter	Content
color	All processes with same color end up in same group
int key	Controls rank in final group
newcomm	Output communicator

Splitting communicators: example

The following splits processes into two groups with ratio 1:2.

```
bool const is_apple = rank % 3 == 0;
SECTION("split 1:3 and keep same process order") {
    MPI_Comm apple_orange;
    MPI_Comm_split(MPI_COMM_WORLD, is_apple ? 0: 1, rank, &apple_orange);

    int nrank, nsize;
    MPI_Comm_rank(apple_orange, &nrank);
    MPI_Comm_size(apple_orange, &nsize);

    int const div = (size - 1) / 3, napples = 1 + div;
    if(is_apple) {
       CHECK(nsize == napples);
       CHECK(nrank == rank / 3);
    } else {
       CHECK(nsize == size - napples);
       CHECK(nrank == rank - 1 - (rank / 3));
    }
}
```

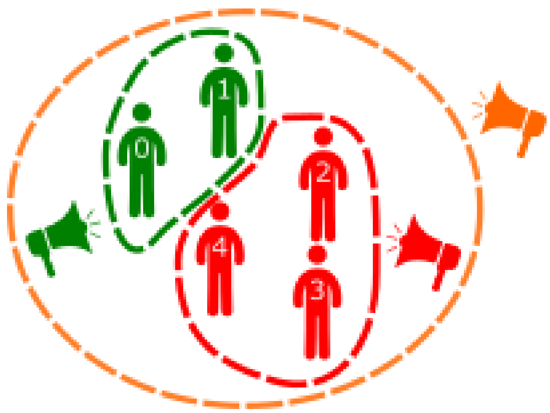
Splitting communicators: Exercise

Exercise:

- use "-rank" as the key: what happens?
- split into three groups with ratios 1:1:2
- use one of the collective operation on a single group

Scatter operation solution

```
std::string const message = "This message is going to come out in separate channels";
```




```
int N = message.size() / size;
if(message.size() < size) return;

char buffer[256];
if(rank == 0) {
  int const error = MPI_Scatter(
          (void*) message.c_str(), N, MPI_CHAR,
          buffer, 256, MPI_CHAR, 0, MPI_COMM_WORLD
  );
  REQUIRE(error == MPI_SUCCESS);
  CHECK(message.substr(rank*N, N) == std::string(buffer, N));
} else {
  int const error = MPI_Scatter(
          NULL, -1, MPI_CHAR, // not significant outside root
          buffer, 256, MPI_CHAR, 0, MPI_COMM_WORLD
  );
  REQUIRE(error == MPI_SUCCESS);
  CHECK(message.substr(rank*N, N) == std::string(buffer, N));
}
```

More advanced MPI

Architecture and usage

- depending on library, MPI processes can be *placed* on specific node…
- … and even chained to specific cores
- Fewer processes than core means we can do MPI + openmp:
- some data is distributed (MPI)
- some data is shared (openMP)

- MPI-3 allows for creating/destroying processes dynamically

Splitting communicators

`MPI_Group_*` specify operations to create sets of processes. In practice, it defines operations on sets:

- union
- intersection
- difference

And allows the creation of a communicator for the resulting group.

More MPI data-types

It is possible to declare complex data types

- strided vectors, e.g. only one of every element (MPI_Type_vector)
- sub-matrices (strided in n axes, n >= 2) (MPI_Type_Create_struct)
- irregular strides (MPI_Type_indexed)

One sided communication

Prior to MPI-3, both sending and receiving processes must be aware of the communication.

One-sided communication allow processes to define a buffer that other processes can access without their explicit knowledge.

And also

- Cartesian grid topology where process (1, 1) is neighbor of (0, 1), (1, 0), (2, 1), (1, 2). With simplified operations to send data EAST, WEST, UP, DOWN. . . .
- More complex graph topologies
- non-blocking collective operations

Chapter 8

MPI Design Example

MPI Design Example

Objectives for this chapter

In this chapter, we give an extended introduction to a particular parallel programming example, introducing some common programming patterns which occur in working with MPI.

Smooth Life

Conway's Game of Life

The Game of Life is a cellular automaton devised by John Conway in 1970.

A cell, on a square grid, is either alive or dead. On the next iteration:

- An alive cell:
  - remains alive if it has 2 or 3 alive neighbours out of 8
  - dies (of isolation or overcrowding) otherwise
- A dead cell:
  - becomes alive if it has exactly 3 alive neighbours
  - stays dead otherwise

Conway's Game of Life

This simple set of rules produces beautiful, complex behaviours:

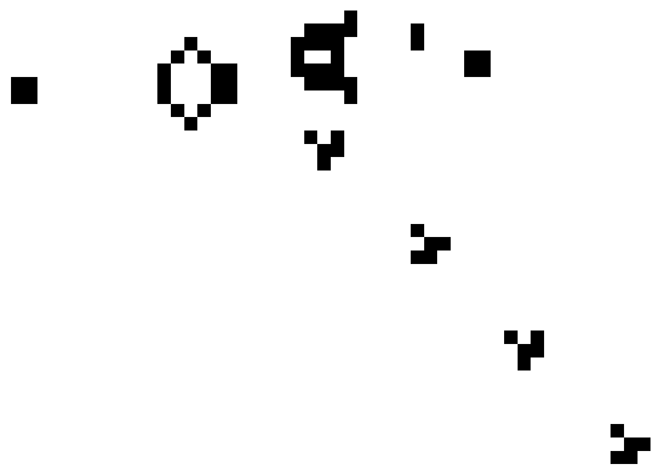


Figure 8.1: "Gospers glider gun" by Kieff. Licensed under CC BY-SA 3.0 via Wikimedia Commons.

Smooth Life

Smooth Life, proposed by Stephan Rafler, extends this to continuous variables:

- The neighbourhood is an integral over a ring centered on a point.
- The local state is an integral over the disk inside the ring.

(The ring has outer radius 3*inner radius, so that the area ratio of 1:8 matches the grid version.)

Smooth Life

- A point has some degree of aliveness.
- Next timestep, a point's aliveness depends on these two integrals. (`$F_{r}$` and `$F_{d}$`)
- The new aliveness `$S(F_{r},F{d})$` is a smoothly varying function such that:
  - If `$F_{d}$` is 1, S will be 1 if `$d_1< F_{r} < d_2$`
  - If `$F_{d}$` is 0, S will be 1 if `$b_1< F_d < b_2$`

A "Sigmoid" function is constructed that smoothly blends between these limits.

Smooth Life on a computer

We discretise Smooth Life using a grid, so that the integrals become sums. The aliveness variable becomes a floating point number.

To avoid the hard-edges of a “ring” and “disk” defined on a grid, we weight the sum by the fraction of a cell that would fall inside the ring or disk:

If the distance d from the edge of the ring is within 0.5 units, we weight the integral by $2d-1$, so that it smoothly various from 1 just inside to 0 just outside.

Smooth Life

Smooth Life shows even more interesting behaviour:

SmoothLifeVideo

- Gliders moving any direction
- “Tension tubes”

Serial Smooth Life

Have a look at our serial implementation of SmoothLife.

We can see that this is pretty slow:

If the overall grid is M by N, and the range of interaction (3* the inner radius), is r, then each time step takes MNr^2 calculations: if we take all of these proportional as we “fine grain” our discretisation (a square domain, and a constant interaction distance in absolute units), the problem grows like N^4!

To make this faster, we’ll need to parallelise with MPI. But let’s look at a few interesting things about the serial implementation.

Main loop

Four levels deep:

```
void Smooth::QuickUpdate() {
  for (int x=0;x<sizex;x++) {
    for (int y=0;y<sizey;y++) {
      double ring_total=0.0;
      double disk_total=0.0;
```

```
      for (int x1=0;x1<sizex;x1++) {
          int deltax=TorusDifference(x,x1,sizex);
          if (deltax>outer+smoothing/2) continue;

          for (int y1=0;y1<sizey;y1++) {
            int deltay=TorusDifference(y,y1,sizey);
            if (deltay>outer+smoothing/2) continue;

            double radius=std::sqrt(deltax*deltax+deltay*deltay);
            double fieldv=(*field)[x1][y1];
            ring_total+=fieldv*Ring(radius);
            disk_total+=fieldv*Disk(radius);
          }
      }

      (*fieldNew)[x][y]=transition(disk_total/normalisation_disk,ring_total/normalisation_ri
    }
  }
```

Swapped before/after fields

```
  std::vector<std::vector<density> > * fieldTemp;
  fieldTemp=field;
  field=fieldNew;
  fieldNew=fieldTemp;
  frame++;
}
```

Distances wrap around a torus

```
int Smooth::TorusDifference(int x1, int x2, int size) const {
    int straight=std::abs(x2-x1);
    int wrapleft=std::abs(x2-x1+size);
    int wrapright=std::abs(x2-x1-size);
    if ((straight<wrapleft) && (straight<wrapright)) {
      return straight;
    } else {
      return (wrapleft < wrapright) ? wrapleft : wrapright;
    }
}
```

Smoothed edge of ring and disk.

```
double Smooth::Disk(distance radius) const {
  if (radius>inner+smoothing/2) {
    return 0.0;
  }
  if (radius<inner-smoothing/2) {
    return 1.0;
  }
  return (inner+smoothing/2-radius)/smoothing;
}
```

Automated tests for mathematics

```
  SECTION ("Sigmoid function is correct") {
    double e=std::exp(1.0);
    REQUIRE(Smooth::Sigmoid(1.0,1.0,4.0) == 0.5);
    REQUIRE(std::abs(Smooth::Sigmoid(1.0,0.0,4.0)-e/(1+e))<0.0001);
    REQUIRE(Smooth::Sigmoid(10000,1.0,4.0) == 1.0);
    REQUIRE(std::abs(Smooth::Sigmoid(0.0,1.0,0.1)) < 0.001);
  }
```

Domain decomposition

Domain decomposition

One of the most important problems in designing a parallel code is “Domain Decomposition”:

- How will I divide up the calculation between processes?

Design objectives in decomposition are:

- Minimise communication
- Optimise load balance (Share out work evenly)

Decomposing Smooth Life

We’ll go for a 1-d spatial decomposition for smooth life, dividing the domain into “Stripes” along the x-axis.

If we have an N by M domain, and p, processes, each process will be responsible for NM/p cells, and NMr^2/p calculations.

Static and dynamic balance

This will achieve perfect **static** load balance: the average work done by each process is the same. If we were not solving in a rectangular grid, this would have been harder.

However, since the calculation can (perhaps) be done quicker when the domain is empty, and our field will vary as time passes, we will not achieve perfect **dynamic** load balance.

Communication in Smooth Life

Given that each cell needs to know the state of cells within a range $r = 3r_d$, where r_d is the inner radius of the neighbourhood ring, and r the outer radius, we need to get this information to the neighbouring sites.

This is *great*: we only need to transfer information to neighbours, not all the other processes. Such "local" communication results in fast code.

The amount of communication to take place each time step is proportional to rMp, but assuming an appropriate network topology exists, each pair of neighbours can look after their communication at the same time, so communication will take time proportional to rMp/p=rM.

Strong scaling

We therefore expect the time taken for a simulation to vary like: $Mr(k + Nr/p)$. (Where k is a parameter describing the relative time to communicate one cell's state compared to the time for calculating one cell)

Thus, we see that for a FIXED problem size, the benefit of parallelism will disappear and communication will dominate: this is Amdahl's law again.

Weak scaling

However, if we consider larger and larger problems, growing N as p grows, then we can stop communication overtaking us. This is a common outcome: *local* problems provide perfect *weak* scaling (until network congestion or IO problems dominate).

Any NONLOCAL communication, where the total amount of time for communication to take place grows as the number of processes does (such as a gather, which takes p, a reduction, like $ln(p)$, or an all-to-all, like p^2, means that perfect weak scaling can't be achieved.)

Halo swap

Where do we put the communicated data?

The data we need to receive from our neighbour needs to be put in a place where it can be conveniently used to calculate the new state of cells within distance r of the boundary.

The standard design pattern for this is to use a **Halo Swap**: we extend the memory buffer used for our state, adding new space either side of our main domain to hold a **halo**.

Domains with a halo

Thus, each process now holds $N + 2r$ cells:

- $0 \leq x < r$, the left halo, holding data calculated by the left neighbour
- $r \leq x < 2r$, data which we calculate, which will form our **left neighbour's right halo**
- $2r \leq x < N$, data which we calculate, unneeded by neighbours
- $N \leq x < N + r$, data which we calculate, which will form our **right neighbour's left halo**
- $N + r \leq x < N + 2r$, the right halo.

Domains with a halo

```
range(outer+smoothing/2),
local_x_size(sizex/mpi_size),
local_x_size_with_halo(local_x_size+2*range),
total_x_size(sizex),
x_coordinate_offset(rank*local_x_size-range),
local_x_min_calculate(range),
local_x_max_needed_left(2*range),
local_x_max_calculate(range+local_x_size),
local_x_min_needed_right(local_x_size),
```

Coding with a halo

We will thus **update** the field only from r to $N+r$, but we will **access** the field from 0 to $N+2r$:

```
int from_x=0; int to_x=local_x_size_with_halo
```

```
void Smooth::QuickUpdateStripe(int from_x,int to_x) {
  for (int x=from_x;x<to_x;x++) {
    for (int y=0;y<sizey;y++) {
      double ring_total=0.0;
      double disk_total=0.0;
      for (int x1=0;x1<local_x_size_with_halo;x1++) {
          int deltax=TorusDifference(x+x_coordinate_offset,x1+x_coordinate_offset,total_x_si
          if (deltax>outer+smoothing/2) continue;

          for (int y1=0;y1<sizey;y1++) {
            int deltay=TorusDifference(y,y1,sizey);
            if (deltay>outer+smoothing/2) continue;

            double radius=std::sqrt(deltax*deltax+deltay*deltay);
            double fieldv=Field(x1,y1);
            ring_total+=fieldv*Ring(radius);
            disk_total+=fieldv*Disk(radius);
          }
      }

      SetNewField(x,y,transition(disk_total/normalisation_disk,ring_total/normalisation_ring
    }
  }
}
```

Transferring the halo

We need to pass data left at the same time as we receive data from the right.

If we use separate `Send` and `Recv` calls, we'll have a deadlock: process 2 will be sending to process 1, while process 3 is sending to process 2. No process will be executing a `Recv`.

Fortunately, MPI provides `Sendrecv`: expressing that we want to do a blocking `Send` to one process while we simultaneously do a blocking `Recv` from another. Exactly what we need for pass-the-parcel.

Transferring the halo

```
void Smooth::CommunicateMPI(){
  BufferLeftHaloForSend();
  MPI_Sendrecv(send_transport_buffer,range*sizey,MPI_DOUBLE,left,rank,
      receive_transport_buffer, range*sizey,MPI_DOUBLE,right,right,
      MPI_COMM_WORLD,MPI_STATUS_IGNORE);
  UnpackRightHaloFromReceive();
  BufferRightHaloForSend();
  MPI_Sendrecv(send_transport_buffer,range*sizey,MPI_DOUBLE,right,mpi_size+rank,
      receive_transport_buffer,range*sizey,MPI_DOUBLE,left,mpi_size+left,
      MPI_COMM_WORLD,MPI_STATUS_IGNORE);
  UnpackLeftHaloFromReceive();
}
```

Noncontiguous memory

Our serial solution uses a C++ `vector<vector<double> >` to store our field.

That means each column of data starts at a different location in memory; our data is not contiguous in memory, the outer vector holds a series of pointers to the start of each inner vector.

This means we can't just transmit Mr `doubles` in one go by sending from the address of `&field1[0][0]`.

Buffering

We'll get around this by copying all the data into a send buffer, and unpacking from a receive buffer. This adds to our communication overhead, but doesn't change its scaling behaviour, both overheads are $O(Mr)$.

We'll look in a later section how this can be avoided.

Buffering

```
void Smooth::BufferLeftHaloForSend(){
  for (int x=local_x_min_calculate; x<local_x_min_calculate+range;x++){
    for (int y=0; y<sizey;y++){
      send_transport_buffer[y*range+x-local_x_min_calculate]=Field(x,y);
    }
  }
}
```

```
void Smooth::UnpackRightHaloFromReceive(){
  for (int x=local_x_max_calculate; x<local_x_size_with_halo;x++){
    for (int y=0; y<sizey;y++){
      SetField(x,y,receive_transport_buffer[y*range+x-local_x_max_calculate]);
    }
  }
}
```

Testing communications

We implement a copy of our buffers which doesn't use MPI:

```
void Smooth::CommunicateLocal(Smooth &left, Smooth &right){
  BufferLeftHaloForSend();
  std::memcpy(left.receive_transport_buffer,send_transport_buffer,sizeof(density)*range*size
  left.UnpackRightHaloFromReceive();
  BufferRightHaloForSend();
  std::memcpy(right.receive_transport_buffer,send_transport_buffer,sizeof(density)*range*siz
  right.UnpackLeftHaloFromReceive();
}
```

which allows us to check our halos are all set up correctly.

Testing communications

We test that our copy works as expected:

```
TEST_CASE ("CommunicationBufferingFunctionsCorrectly") {
  Smooth smooth(200,100,5,0,2);
  Smooth smooth2(200,100,5,1,2);
  REQUIRE(smooth.LocalXSize()==100);
  REQUIRE(smooth.LocalXSizeWithHalo()==130);
  REQUIRE(smooth.Radius(0,0,0,0)==0);
  REQUIRE(smooth2.Radius(0,0,0,0)==0);
  smooth.SeedDisk(); // Half the Seeded Disk falls in smooth2's domain, so total filling wi
  REQUIRE(smooth.Field(15,0)==1.0);
  REQUIRE(std::abs(smooth.FillingDisk(15,0)-0.5)<0.1);
  REQUIRE(smooth2.FillingDisk(85,0)==0.0);
  smooth.CommunicateLocal(smooth2,smooth2); // Transport the data
  REQUIRE(std::abs(smooth.FillingDisk(15,0)-0.5)<0.1);
```

```
  REQUIRE(smooth2.Field(115,0)==1.0);
  REQUIRE(std::abs(smooth2.FillingDisk(115,0)-0.5)<0.1);
}
```

Testing communications

We test that the MPI comms results are the same as serial

```
      smooth.QuickUpdate();
      paraSmooth.CommunicateMPI();
      paraSmooth.QuickUpdate();
      paraSmooth.CommunicateMPI();
      for (unsigned int x=0;x<50;x++){
        for (unsigned int y=0;y<100;y++){
          REQUIRE(std::abs(smooth.Field(x+15+rank*50,y) - paraSmooth.Field(x+15,y))<0.00001
        }
      }
    }
```

Deployment

Getting our code onto Legion

We now have to

- Clone our code base onto our cluster
- Load appropriate modules to get the compilers we need
- Build our code
- Construct an appropriate submission script
- Submit the submission script
- Wait for the job to queue and run
- Copy the data back from the cluster
- Analyse it to display our results.

This is a **pain in the neck**

Scripting deployment

There are various tools that can be used to automate this process.

You should use one.

Since I like Python, I use Fabric to do this.

You create `fabfile.py` in your top level folder, and at the shell you can write:

```
fab legion.cold
fab legion.sub
fab legion.stat
fab legion.fetch
```

to build and run code on Legion, without ever using ssh. You can be in any folder below the `fabfile.py` level, such as inside a build folder; the command line tool recurses upward to look for this file, (Just like `git` looks for the `.git` folder.)

Writing fabric tasks

If you know Python, writing fabric tasks is easy:

fabfile.py:

```
@task
def build():
    with cd('/home/ucgajhe/smooth/build'):
        with prefix('module load cmake'):
            run('make')
```

```
fab build
```

Templating jobscripts

Editing a jobscript every time you want to change the number of cores you want to run on is tedious. I use a templating tool Mako to generate the jobscript:

```
#$ -pe openmpi ${processes}
```

the templating tool fills in anything in ${} from a variable in the fabric code.

Mako Template for Smooth Life

Configuration files

Avoid using lots of command line arguments to configure your program. It's easier to just have one argument, a configuration file path.

- The configuration file can be kept with results for your records.
- Configuration files can be shipped back and forth to the cluster with fabric.

Even if your code is using simple C++ I/O rather than a nice formatting library, it's best to design your config file in a format which other frameworks can easily read. My favourite is Yaml.

```
width: 200
height: 100
range: 5
```

Results

It works

Derived Datatypes

Avoiding buffering

We've still got our ugly re-buffering of the halo data into contiguous memory, arising from our use of `vector<vector< double > >`

We can get around that by changing to a flat 1-d array of memory, and storing the (x, y) element at `Field[`$Mx + y$`]`. This works fine, especially if we refactor all access to get and update from the field into accessors, so we only need make the change in one place.

Wrap Access to the Field

```
density Smooth::Field(int x,int y) const {
  return (*field)[sizey*x+y];
};

void Smooth::SetNewField(int x, int y, density value){
  (*fieldNew)[sizey*x + y]=value;
}
```

```
void Smooth::SetField(int x, int y, density value){
  (*field)[sizey*x + y]=value;
}

void Smooth::SeedField(int x, int y, density value){
  SetField(x,y,value+Field(x,y));
  if (Field(x,y)>1.0){
     SetField(x,y,1.0);
  }
}
```

Copy Directly without Buffers

```
void Smooth::CommunicateMPIUnbuffered(){
  MPI_Sendrecv((*field)+sizey*range,range*sizey,MPI_DOUBLE,left,rank,
      (*field)+sizey*local_x_max_calculate, range*sizey,MPI_DOUBLE,right,right,
      MPI_COMM_WORLD,MPI_STATUS_IGNORE);
  MPI_Sendrecv((*field)+sizey*local_x_min_needed_right,range*sizey,MPI_DOUBLE,right,mpi_size
      (*field),range*sizey,MPI_DOUBLE,left,mpi_size+left,
      MPI_COMM_WORLD,MPI_STATUS_IGNORE);
}
```

Defining a Halo Datatype

It's usually the case in programming that thinking of a whole body of data as a single entity produces cleaner, faster code than programming at the level of the individual datum.

We want to be able to think of the *Halo* as a single object to be transferred, rather than as a series of `doubles`.

We can do this using an MPI Derived Datatype:

Declare Datatype

```
void Smooth::DefineHaloDatatype(){
  MPI_Type_contiguous(sizey*range,MPI_DOUBLE,&halo_type);
  MPI_Type_commit(&halo_type);
}
```

Use Datatype

```
void Smooth::CommunicateMPIDerivedDatatype(){
  MPI_Sendrecv(*field+sizey*local_x_min_calculate,1,halo_type,left,rank,
               *field+sizey*local_x_max_calculate,1,halo_type,right,right,
               MPI_COMM_WORLD,MPI_STATUS_IGNORE);
  MPI_Sendrecv(*field+sizey*local_x_min_needed_right,1,halo_type,right,mpi_size+rank,
                                                *field,1,halo_type,left,mpi_size+left,
                                                MPI_COMM_WORLD,MPI_STATUS_IGNORE);
}
```

Strided datatypes

Supposing we wanted to use a 2-d decomposition. Our y-direction halo's data would not be contiguous in memory.

Let's imagine we used $Ny + x$ to index into the field instead of $Mx + y$: we can define a derived datatype which specifies data as a series of stretches, with gaps.

`MPI_Type_Vector(`M, r, N`)` would define the relevant type for this: M chunks, each r `double`s long, each N `double`s apart in memory.

Overlapping computation and communication

Wasteful blocking

We are calculating our whole field, then sharing all the halo.

This is wasteful: we don't need our neighbour's data to calculate the data in the *middle* of our field.

We can start transmitting our halo and receiving our neighbour's, while calculating our middle section. Thus, our communication will not take up extra time, as it is overlapped with calculation.

To do this, we need to use asynchronous communication.

Asynchronous communication strategy

- Start sending/receiving data
- Do the part of calculation independent of needed data
- Wait until the communication is complete (hopefully instant, if it's already finished)
- Do the part of the calculation that needs communicated data

Asynchronous communication for 2-d halo:

- Start clockwise send/receive
- Calculate middle
- Finish clockwise send
- Start anticlockwise send
- Calculate right
- Finish anticlockwise send
- Calculate left

Asyncronous MPI

```
void Smooth::InitiateLeftComms(){
  MPI_Isend(*field+sizey*local_x_min_calculate,1,halo_type,left,rank,MPI_COMM_WORLD,&request
  MPI_Irecv(*field+sizey*local_x_max_calculate,1,halo_type,right,right,MPI_COMM_WORLD,&reque
}


void Smooth::ResolveLeftComms(){
  MPI_Wait(&request_left,MPI_STATUS_IGNORE);
}
```

Implementation of Asynchronous Communication

```
void Smooth::UpdateAndCommunicateAsynchronously(){

  InitiateLeftComms();
  // Calculate Middle Stripe
  QuickUpdateStripe(local_x_max_needed_left,local_x_min_needed_right);
  ResolveLeftComms(); // So we now have the right halo
  InitiateRightComms();
  QuickUpdateStripe(local_x_min_needed_right,local_x_max_calculate);
  ResolveRightComms();
  QuickUpdateStripe(local_x_min_calculate,local_x_max_needed_left);
  SwapFields();
}

density * Smooth::StartOfWritingBlock(){
   return &(*field)[local_x_min_calculate*sizey];
}
```

Chapter 9

MPI File I/O

Parallel Input and Output

Objectives for the Chapter

In this chapter, we discuss how to get information *out* of our parallel programs, and how to configure them.

Because we need to reconcile the outputs from different processes, and distribute configuration amongst them, this can be quite complex.

We will look at a few different choices of how to do this.

Visualisation

Visualisation is important

We've put a lot of emphasis onto using **Unit Tests** to verify your code.

However, it's just as important to *visualise* your results.

"The graph looks OK" is not a good enough standard of truth.

But "the graph looks wrong" is a strong indication of problems!

Visualisation is hard

Three-D slices through your data, contour surfaces, animations…

These are all really important for understanding scientific output.

But doing the visualisation in C++ can be very very difficult.

Simulate remotely, analyse locally

Visualise locally if you can.

Use a tool like fabric to organise your data and make it easy to ship it back from the cluster.

Use dynamic languages like Python or Matlab to visualise your data, or tools like Paraview or VisIt.

In-Situ visualisation

When working at the highest scales of parallel, saving out raw simulation data becomes impossible: compute power scales faster than storage.

Under these circumstances, it is necessary to do **data reduction** on the cluster.

In-situ visualisation, where animations or graphs are constructed as part of the analysis, is one approach.

Visualising with NumPy and Matplotlib

The Python toolchain for visualising quantitative data is powerful, fast and easy.

Here's how we turn a NumPy Matrix view of our data, with axes (frames, width, height), into an animation and save it to disk as an mp4:

```
import matplotlib.animation
import matplotlib.pyplot
def plot(frames,outpath):
    figure = matplotlib.pyplot.figure()
    def _animate(frame_id):
        print "Processing frame", frame_id
        matplotlib.pyplot.imshow(frames[frame_id], vmin=0, vmax=1)

    anim = matplotlib.animation.FuncAnimation(figure, _animate, len(frames), interval=100)
    anim.save(outpath)
```

Try doing that with C++ libraries!

Formatted Text IO

Formatted Text IO

- Is easy

- Is portable
- Is human-readable
- Is slow
- Wastes space

When and when not to use text IO

Use text IO:

- Metadata
- Configuration
- Logging

Don't use it:

- For output of large numerical datasets
- For initial conditions
- For checkpoint/restart

Use libraries to generate formatted text

For a templating library like Mako in C++ try CTemplate

This is a great way to create XML and YAML files.

Raw CSV file generation with built-in C++ `<iostream>` is not very robust.

Libraries will automatically quote strings which contain commas.

Boost's Spirit library is good for this too.

Low-level IO exemplar

Nevertheless, in simple cases where text is of a known format, C++'s built in formatted IO is quick and easy:

```
void TextWriter::Header(int frames){
  *outfile << smooth.LocalXSize() << ", " << smooth.Sizey() << ", " << rank << ", " << size
}
```

```
void TextWriter::Write() {
   for (int x=smooth.Range();x<smooth.LocalXSize()+smooth.Range();x++) {
     for (int y=0;y<smooth.Sizey();y++) {
        *outfile << smooth.Field(x,y) << " , ";
     }
     *outfile << std::endl;
   }
   *outfile<< std::endl;
}
```

Text Data and NumPy

Parsing text data in NumPy is also very easy:

```
buffer=numpy.genfromtxt(data,delimiter=",")[:,:-1]
```

```
frames_data=buffer.reshape([frame_count, width/size, height])
```

this is how the animations you saw last lecture were created.

Text File Bloat

However, representing $1.3455188104 \cdot 10^{-10}$ in text:

```
1.3455188104e-10,
```

uses many bytes per number, (one per character in ASCII, more in unicode) whereas recording in a binary representation, even at double precision, typically uses 8.

It's also harder do parallel IO in such files, as the distance of a certain quantity from the start of the file can't be predicted.

Binary IO in C++

Binary IO in C++

To do basic binary file IO in C++, we set `std::ios::binary` as we open the file.

However, we can't use the nice `<<` operator, as these still generate formatted `char`s. We have to use `ostream::write()`, which is a low-level, C-style function.

Binary IO in C++

```
void BinaryWriter::Header(int frames){
  outfile->write(reinterpret_cast<char*>(&sizex),sizeof(int));
  outfile->write(reinterpret_cast<char*>(&sizey),sizeof(int));
  outfile->write(reinterpret_cast<char*>(&rank),sizeof(int));
  outfile->write(reinterpret_cast<char*>(&size),sizeof(int));
  outfile->write(reinterpret_cast<char*>(&frames),sizeof(int));
}
```

```
void BinaryWriter::Write() {
  outfile->write(reinterpret_cast<char*>(smooth.StartOfWritingBlock()),
      local_element_count*sizeof(double));
}
```

Binary IO in NumPy

```
buffer = numpy.fromfile(data, bulk_type, frame_count*height*width/size)
```

... more on that 'bulk_type' parameter later.

Endianness and Portability

Portability

There's a big problem with binary files: the bytes that get written for a `double` on one platform are different from those on others.

This is particularly problematic in HPC: the architecture of your laptop is unlikely to be the same as on ARCHER, so if when ship your output files back, your nice visualisation code will not work.

Length of datatypes

The C++ standard **does not** specify how many bytes are used to represent a `double`: just that it is more than a `float`! (And similarly for other datatypes.)

This means that your data will be represented differently on different platforms.

Therefore, don't forget to use `sizeof(type)` whenever working with byte-level routines like MPI, if you want your code to work on both your laptop, and your local supercomputer.

Endianness

Another problem is Endianness: a `double` is actually **almost** always 8 bytes, with a 1 bit sign, 11 bit exponent, and 52 bit mantissa. (The IEEE standard).

But there's still ambiguity in how these bytes are ordered.

The 4-byte standard signed integer "5" can be represented as:

> 00000101 00000000 00000000 00000000 (little endian)

or as

> 00000000 00000000 00000000 00000101 (big endian)

NumPy dtypes

As long as you're aware of these problems, you can usually make your visualiser compatible with the endianness and byte counts of the data you're getting off your system.

If you're visualising with python you can set your datatype to be e.g. `<f8` for a little endian 8-byte floating point, or `>i4` for a big-endian 4-byte signed integer.

XDR

XDR, or 'extensible data representation' is a portability standard defined for binary IO. If you write through XDR, data will be converted to the XDR standard representation.

XDR data is big endian, has everything in multiples of 4 bytes, and supports a rich library of appropriate types.

Writing with XDR

```
#include <cstdio>
#include <rpc/types.h>
#include <rpc/xdr.h>


void XDRWriter::Write() {

  char * start_to_write=reinterpret_cast<char*>(smooth.StartOfWritingBlock());
  xdr_vector(&xdrfile,start_to_write,local_element_count,sizeof(double),reinterpret_cast<xdr
}
```

```
xdrstdio_create(&xdrfile, myFile, XDR_ENCODE);
```

Writing from a single process

One process, one file

So far, we've been writing one process from each file, calling them `frames.dat.0`, `frames.dat.1` etc.

```
fname << "." << rank << std::flush;
```

We've then been reconciling them together in our visualiser code:

```
def append_process_suffix(prefix, process):
    return prefix + '.' + str(process)

def process_many_files(folder, prefix, size, header_type, bulk_type):


    process_frames=[]
    for process in range(size):
        path=os.path.join(folder,append_process_suffix(prefix,process))


    return numpy.concatenate(process_frames, 1)
```

One process, one file

This is necessary, because we **cannot** simply have multiple processes writing to the same file, without considerable care, as they will:

- Block while waiting for access to the file
- Overwrite each others' content

However, the one-process-one-file approach **does not scale** to large numbers of files: the file system can be overwhelmed once we're running at the thousands-of-processors level.

Writing from a single process

An alternative approach is to share all the data to a master process. (Which can be done in $O(lnp)$ time), and then write from that file.

This avoids the complexity of reconciling datafiles locally, and avoids overwhelming the cluster filesystem with many small files.

Writing from a single process

```
void SingleWriter::Write() {

  double * receive_buffer;

  if (rank==0){
     receive_buffer=new double[total_element_count];
  }

  MPI_Gather(smooth.StartOfWritingBlock(),local_element_count,MPI_DOUBLE,
      receive_buffer,local_element_count,MPI_DOUBLE,0,MPI_COMM_WORLD);

  if (rank==0){
     xdr_vector(&xdrfile,reinterpret_cast<char*>(receive_buffer),
         total_element_count,sizeof(double),reinterpret_cast<xdrproc_t>(xdr_double));
  }
}
```

Writing from a single process

It's important to create the file and write the header only on the master process:

```
SingleWriter::SingleWriter(Smooth & smooth, int rank, int size)
    :SmoothWriter(smooth,rank,size)
{
     if (rank!=0) {
       return;
     }
```

Parallel IO

Serialising on a single process

We know that *any task which is not $O(1/p)$ will eventually dominate the cost as number of processes increases, preventing scaling.

This is Amdahl's law again.

The master-process-writes approach introduces this problem; IO quickly becomes the dominant part of the task, preventing weak scaling as problem sizes and processor counts increase.

Parallel file systems

Supercomputers provide **parallel file systems**. These store each file in multiple "stripes": one can obtain as much parallelism in IO as there are stripes in files.

To make use of this, it is necessary to use MPI's parallel IO library, MPI-IO.

Introduction to MPI-IO

MPI-IO works by accessing files as data buffers like core MPI_Send and so on:

```
MPI_File_write(outfile,smooth.StartOfWritingBlock(),local_element_count,MPI_DOUBLE,MPI_STA
```

Opening parallel file

All processes work together to open and create the file:

```
MPI_File_open(MPI_COMM_WORLD, const_cast<char *>(fname.str().c_str()),
              MPI_MODE_CREATE | MPI_MODE_RDWR, MPI_INFO_NULL, &outfile);
```

Finding your place

The hard part is synchronising things so that each process writes it's section of the file:

```
int offset=4*sizeof(int) + // The header
           rank*local_element_count*sizeof(double) + // Offset within the frame
           smooth.Frame()*total_element_count*sizeof(double); // Frame offset in the file

MPI_File_seek(outfile,offset,MPI_SEEK_SET);
```

High level research IO libraries

Standard libraries for scientific data formats such as HDF5 support parallel IO.

You should use these if you can, as you'll get the benefits of both endianness-portability and parallel IO, together with built-in metadata support and compatibility with other tools.

Introduction to HDF5 or NetCDF is beyond the scope of this course, but familiarising yourself with these is strongly encouraged!

Chapter 10

Accelerators

Introduction to Accelerators

What is an accelerator?

- An accelerator is a piece of computing hardware that performs some function faster than is possible in software running on a general purpose CPU
  - an example is the Floating Point Unit inside a CPU that performs calculations on real numbers faster than the Arithmetic and Logic Unit
  - better performance is achieved through concurrency - the ability to perform several operations at once, in parallel
- When an accelerator is separate from the CPU it is referred to as a "hardware accelerator"

Why would I want to use one?

- Accelerators are designed to execute domain-specific computationally intensive software code faster than a CPU
  - 3D graphics
  - MPEG decoding
  - cryptography

Vectorisation

Using an accelerator within the CPU

- Consider the following code which performs `y = a*x + y` on vectors `x` and `y`:

```
int saxpy(int n, float a, const float * restrict x, int incx,
          float * restrict y, int incy) {
    if (n < 0)
        return 1;

    for (int i = 0; i < n; i++)
        y[i * incy] += a * x[i * incx];

    return 0;
}
```

- Assuming single precision floating point multiply-add is implemented as one CPU instruction the `for` loop executes `n` instructions (plus integer arithmetic for the loop counter, etc.).

CPUs as multicore vector processors

- In the mid-1990s, Intel were investigating ways of increasing the multimedia performance of their CPUs without being able to increase the clock speed
- Their solution was to implement a set of registers capable of executing the same operation on multiple elements of an array in a single instruction
  - known as SIMD (Single Instruction, Multiple Data)
  - branded as MMX (64-bit, integer only), SSE (128-bit, integer + floating point) and AVX (256-bit)

Compiler Autovectorisation

- Modern compilers are able to automatically recognise when SIMD instructions can be applied to certain loops
  - elements are known to be contiguous
  - arrays are not aliased

```c
int saxpy_fast(int n, float a, const float * restrict x, int incx,
               float * restrict y, int incy) {
    if (n < 0)
        return 1;

    if (incx == 1 && incy == 1) {
        for (int i = 0; i < n; i++)
            y[i] += a * x[i];
    }
    else {
        for (int i = 0; i < n; i++)
            y[i * incy] += a * x[i * incx];
    }

    return 0;
}
```

Autovectorisation results

- Running this and timing the invocations produces the following output:

```
n = 10000, incx = 1, incy = 1
saxpy: 0.008052ms
saxpy_fast: 0.002845ms
```

- Since Intel's SIMD registers operate on 4 single precision floats at once the first loop executes approximately `n/4` instructions
  - resulting in a (near) 4x speedup (Amdahl's Law)
- Can be combined with OpenMP directives (lecture 5) to use SIMD units on multiple cores of the CPU

Support for Autovectorisation

- GCC
  - use `-ftree-loop-vectorize` to activate
  - use `-fopt-info-vec` to check whether loops are vectorised
  - automatically performed with `-O3`
- ICC
  - use `-vec` (Linux/OSX) or `/Qvec` (Windows) to activate

  - use `-vec-report=n`/`/Qvec-report:n` to check whether loops are vectorised (`n > 0`)
  - automatically performed with `-O2`/`/O2` and higher

Support for Autovectorisation

- Clang
  - use `-fvectorize` to activate
  - automatically performed at `-O2` and higher
  - no way to see compiler auto-detection
- MSVC
  - activated by default
  - use `/Qvec-report:n` to check whether loops are vectorised (`n > 0`)

Using a GPU as an Accelerator

GPUs for 3D graphics

- 3D graphics rendering involves lots of operations on 3 and 4 dimensional vectors
  - positions of vertices (x, y, z)
  - colour and transparency of pixels (RGBA)
- Realtime graphics rendering needs to be fast so accuracy is often sacrificed
  - GPUs are good at 32-bit integer and single precision floating point arithmetic
  - not as good at 64-bit integer and double precision floating point
- 3D graphics operations are independent of one another
  - and can be performed in parallel

GPUs as multicore vector processors

- GPUs are multicore vector processors.
- They have much faster memory access to their own memory
- And very slow transfer (more like 'download') to the main processor (~5GB/s)
- They have *much* slower single-core performance (but you would never do this)

Property	CPU	GPU
No of cores	<10	1000s
SIMD width	256 bits	1024 bits
Memory bandwidth	<25 GB/s	<500 GB/s

GPU Hardware

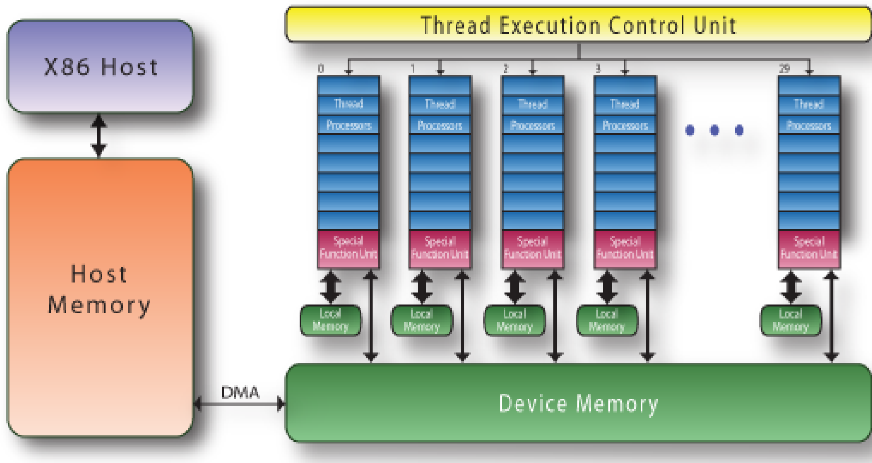
- Each core (multiprocessor - often abbreviated as "SM" or "MP") has:
  - 128 Single Precision Floating Point Units
  - 32 Double Precision FPUs (that also perform single precision transcendental functions)
  - 16384 32-bit registers (very fast access)
  - 64KB of "shared" cache memory (fast access)
  - 10KB of "constant" cache memory (writable by the CPU, fast, read-only access by the GPU)
- GPUs also have "global" memory which is the figure quoted by graphics card manufacturers (2GB, etc.)
  - accessed by the CPU across the PCI-Express bus
  - high latency, slow access by the GPU (but still up to 20x faster than CPU RAM access)

General Purpose Programming for GPUs

- GPU threads are run in (up to) 3-dimensional groups called "blocks"
- Each block runs on one SM
  - threads within a block can communicate via shared memory and use barrier synchronisation
- Threads have their own registers for local variables
- Each SM executes blocks of threads in groups of 32 called a "warp"

GPU Architecture

See more



SIMT

- Multiple thread blocks are arranged in a 3-dimensional "grid"
- No communication/synchronisation primitives across blocks/SMs
  - can use atomic operations on variables in global memory (slow)
- This type of programming is a hybrid between threaded programming and SIMD and hence is called SIMT by Nvidia

Executing code on the GPU

- Functions executed on the GPU and called from the CPU are called "kernels"
  - kernel execution is asynchronous to the CPU
  - CPU must call a function which blocks until the GPU has finished executing the current kernel before attempting to download results
  - there is an implicit synchronisation barrier on the GPU at the start of each kernel
- Common programming pattern:
  - upload data from CPU RAM to GPU global memory (slow)
  - execute kernel(s) on GPU (fast)
  - synchronise
  - download results (slow)

GPU-accelerating your code

- Four options to GPU accelerate code:
  - replace existing libraries with GPU-accelerated ones
  - use compiler directives to automatically generate GPU-accelerated portions of code
  - use CUDA::Thrust C++ template library to build your own kernels
  - write your own kernels in CUDA-C

GPU-accelerated Libraries

CUDA Libraries

- There are GPU-accelerated libraries available for:
  - random number generation
  - fast Fourier transforms
  - BLAS/LAPACK
  - sparse linear algebra
- Nvidia ships cuRAND, cuFFT and cuBLAS with the CUDA toolkit
  - 3rd party alternatives including MAGMA

Converting existing code

- Each library contains pre-written GPU kernels implementing common operations optimised for several classes of GPU
- All that is required is to convert existing code that calls a CPU library to follow the upload/execute/synchronise/download pattern
  - allocate GPU memory and upload data using the CUDA runtime library
  - execute pre-written kernel from the specific CUDA library required
  - synchronize, download results and free GPU memory using the CUDA runtime library

SAXPY from cuBLAS

- The following code snippet replaces the `saxpy_fast` function with the equivalent `cublasSaxpy`:

```
    // Allocate vectors on GPU
    float * dx, * dy;
    CUDA_ERROR_CHECK(cudaMalloc((void **)&dx, n * incx * sizeof(float)));
    CUDA_ERROR_CHECK(cudaMalloc((void **)&dy, n * incy * sizeof(float)));

    // Create CUBLAS handle
    cublasHandle_t handle;
    CUBLAS_ERROR_CHECK(cublasCreate(&handle));

    // Copy vectors into GPU memory
    CUBLAS_ERROR_CHECK(cublasSetVector(n, sizeof(float), x, incx, dx, incx));
    CUBLAS_ERROR_CHECK(cublasSetVector(n, sizeof(float), y, incy, dy, incy));

    // Perform the GPU SAXPY
    CUBLAS_ERROR_CHECK(cublasSaxpy(handle, n, &a, dx, incx, dy, incy));

    // Copy results back into CPU memory
    CUBLAS_ERROR_CHECK(cublasGetVector(n, sizeof(float), dy, incy, y, incy));
```

```
n = 10000, incx = 1, incy = 1
saxpy: 0.010205ms
saxpy_fast: 0.002530ms
```

Why isn't it faster?

- GPUs have about 100x the computing power of a CPU
  - but only 20x the memory bandwidth
  - and data transfer over the PCI bus is sloooow.
- SAXPY performs one floating point operation for each element in memory
  - the performance is bound by the memory bandwidth
- Matrix Multiply (SGEMM), however, performs `2k` operations per element
  - matrix multiply: `C = a*A*B + b*C`
  - `A` is `m` by `k`
  - `B` is `k` by `n`
  - `C` is `m` by `n`

SGEMM from cuBLAS

- CUBLAS contains an SGEMM function:

```
    // Allocate matrices on GPU
    float * dA, * dB, * dC;
    size_t dlda, dldb, dldc;
    CUDA_ERROR_CHECK(cudaMallocPitch((void **)&dA, &dlda, m * sizeof(float), k));
    CUDA_ERROR_CHECK(cudaMallocPitch((void **)&dB, &dldb, k * sizeof(float), n));
    CUDA_ERROR_CHECK(cudaMallocPitch((void **)&dC, &dldc, m * sizeof(float), n));

    // cudaMallocPitch returns leading dimensions in bytes while CUBLAS expects
    // them as number of elements
    dlda /= sizeof(float);
    dldb /= sizeof(float);
    dldc /= sizeof(float);

    // Create CUBLAS handle
    cublasHandle_t handle;
    CUBLAS_ERROR_CHECK(cublasCreate(&handle));

    // Copy matrices into GPU memory
    CUBLAS_ERROR_CHECK(cublasSetMatrix(m, k, sizeof(float), A, lda, dA, dlda));
    CUBLAS_ERROR_CHECK(cublasSetMatrix(k, n, sizeof(float), B, ldb, dB, dldb));
    CUBLAS_ERROR_CHECK(cublasSetMatrix(m, n, sizeof(float), C, ldc, dC, dldc));

    // Perform the GPU SGEMM
    CUBLAS_ERROR_CHECK(cublasSgemm(handle,
                                   CUBLAS_OP_N, CUBLAS_OP_N,
                                   m, n, k,
                                   &a, dA, dlda, dB, dldb,
                                   &b, dC, dldc));

    // Copy results back into CPU memory
    CUBLAS_ERROR_CHECK(cublasGetMatrix(m, n, sizeof(float), dC, dldc, C, ldc));
```

```
m = 320, n = 640, k = 640
Bandwidth: 977.532GB/s
Throughput: 244.383GFlops/s
```

Using Compiler Directives

OpenACC

- OpenACC is a set of compiler directives that execute blocks of code on an accelerator

- not specific to GPUs
  - also works with APU (AMD), Xeon Phi (Intel), etc.
- Set of compiler `#pragma`s to specify:
  - blocks of code to be run on an accelerator
  - data movement between host and accelerator
- Similar to OpenMP
  - doesn't modify existing code
  - is ignored by compilers that don't support it
- Requires compiler support
  - pgic (non-free, activate with `-acc` flag)
  - gcc support coming

OpenACC Pragmas

- `#pragma acc kernels` specifies a block of code to be run in parallel on an accelerator
  - uses a lot of autodetection
- `#pragma acc data` specifies data movement between host and accelerator
  - can be used to control data movement between kernel calls
- Each pragma can be customised with clauses that appear at the end of the line
  - `#pragma acc <pragma> [clause...]`

OpenACC Pragma Clauses

- `if(condition)`
  - executes only if the condition evaluates to true
  - falls back to CPU code otherwise
  - can be applied to both kernels and data pragmas among others

Clauses specific to pragma acc kernel

- `num_gangs(n)`
  - specifies the number of thread blocks to use
- `num_workers(n)`

  - specifies the number of threads to use in each block

- `reduction(op, val)`
  - performs a reduction using the specified operator and initial value
  - similar to OpenMP's `reduce` pragma

General clauses for data movement

- `copy(var1,var2,...)`
  - allocates and copies variables from the host to the accelerator before a block
  - copies variables back to the host and deallocates after a block
- `copyin(var1,var2,...)` and `copyout(var1,var2,...)`
  - copies data onto the accelerator at the start of a block or off the accelerator at the end of a block
- `create(var1,var2,...)`, `delete(var1,var2,...)`
  - allocates variables on the accelerator at the start of a block and deallocates them at the end
  - useful for temporary arrays
- `present(var1,var2,...)`
  - variable is already present on device so don't allocate or copy
  - also available as `present_or_copy`, `present_or_create`, `present_or_copyin`, `present_or_copyout`
- `private(var1,var2,...)`
  - variable is copied to each thread (similarly to OpenMP's `private`)

OpenACC SAXPY

- The following code snippet implements a SAXPY kernel using OpenACC:

```
void saxpy(int n, float a, const float * x, int incx, float restrict * y, int incy) {
#pragma acc kernels
  for (int i = 0; i < n; ++i)
    y[i * incy] = a * x[i * incx] + y[i * incy];
}
```

- The only pragma required is the `kernels` pragma which turns the `for` loop into a GPU kernel

OpenACC SGEMM

- OpenACC can also be used to implement an SGEMM kernel:

```
void sgemm(int m, int n, int k,
           float a, const float * restrict A, int lda, const float * restrict B, int ldb,
           float b, float restrict * C, int ldc) {
#pragma acc kernels
  for (int j = 0; j < n; j++) {
      for (int i = 0; i < m; i++)
          C[j * ldc + i] *= b;

      for (int l = 0; l < k; l++) {
          const float temp = a * B[j * ldb + k];
          for (int i = 0; i < m; i++)
              C[j * ldc + i] += temp * A[l * lda + i];
      }
  }
}
```

Further Information

- Further information (documentation/tutorials) is available on the (OpenACC website)[http://www.openacc-standard.org/]

CUDA Thrust

CUDA Thrust

- CUDA Thrust is a C++ template library of parallel algorithms and data structures based on the STL
  - sort, scan, transform and reduction algorithms
  - uses `host_vector` and `device_vector` templated types modelled on `std::vector`
  - supports GPUs via CUDA and CPUs via OpenMP through the same interface
  - all headers in the `thrust` subdirectory
  - all data structures and algorithms declared in the `thrust` namespace
- Open source using the Apache License
  - supplied with the Nvidia CUDA Toolkit
  - source code on GitHub

Vector types

- `template <class T> class thrust::host_vector`
  - declared in `#include <thrust/host_vector.h>`
  - similar to `std::vector` using CPU memory
- `template <class T> class thrust::device_vector`
  - declared in `#include <thrust/device_vector.h>`
  - similar to `std::vector` but using GPU memory

Vector types: Constructors

- The following code fragment shows the three constructors available for `host_vector`

```
// Creates an empty host vector to store double values
thrust::host_vector<double> F;

// Creates a host vector with space for 4 integers
thrust::host_vector<int> H(4);

// Creates a host vector containing 8 floats each initialised to 2.5
thrust::host_vector<float> J(8, 2.5);
```

- `device_vector`s have the same constructors but with storage allocated in GPU memory

Vector types: Copy Constructors

- There are four copy constructors for both `device_vector` and `host_vector`
  - copy from a vector of the same template type

```
thrust::host_vector<int> H1;
thrust::host_vector<int> H2(H1);

- copy from a vector of a different template type


thrust::host_vector<float> H(5);
thrust::host_vector<double> D(H);
```

```
- copy a device_vector from a host_vector (or vice versa)


thrust::host_vector<int> H;
thrust::device_vector<int> D(H);


- create a copy of an STL vector


std::vector<int> stl_vector;
thrust::device_vector<int> D(stl_vector);
```

- Each copy constructor also has a corresponding assignment operator

Vector types: Accessors

- The `[]` operator has been overloaded for `device_vector` and `host_vector`

```
thrust::device_vector<int> D(4,0);
D[0] = 99;
D[1] = 88;
```

- Be careful when accessing the elements of a `device_vector` from host code as each one performs a transfer from GPU memory

Algorithms

- In addition to the two vector data types, Thrust also implements several templated algorithms
  - transform
  - reduce
  - transform_reduce
  - sort
  - search

Algorithms: transform

- The transform algorithm is declared in `thrust/transform.h`

```
thrust::device_vector<int> X(10);
thrust::device_vector<int> Y(10);

// initialize X to 0,1,2,3, ....
thrust::sequence(X.begin(), X.end());

//compute Y = -X
// thrust::transform(first, last, result, unary_op);
thrust::transform(X.begin(), X.end(), Y.begin(), thrust::negate<int>());
```

- `transform` applies a unary_op functor to the elements between `first` and `last` and stores them in `result`

Algorithms: reduce

- The reduction algorithm is declared in `thrust/reduce.h`

```
thrust::device_vector<int> vec(5,1);
//thrust::reduce(first, last, init, binary_op);
int sum = thrust::reduce(D.begin(), D.end(), (int) 0, thrust::plus<int>());
```

- `reduce` applies a `binary_op` functor to the elements between `first` and `last` starting with `init` and returns the result

Algorithms: transform/reduce

- The transform/reduce algorithm is declared in `thrust/transform_reduce.h`
  - it combines the transform and reduce algorithms
  - first elements are transformed using `unary_op`
  - then reduced using `binary_op`

```
thrust::device_vector<int> d(5)
thrust::negate<float> unary_op;
thrust::plus<float> binary_op;
float init = 0;

thrust::transform_reduce(d.begin(), d.end(), unary_op, init, binary_op)
```

Thrust SAXPY

- We can use the `transform` algorithm from Thrust to implement our SAXPY kernel

```
struct saxpy_functor : public thrust::binary_function<float, float, float> {

    const float a;

    saxpy_functor(float _a) : a(_a) {}

    __host__ __device__ float operator()(const float &x, const float &y) const {
        return a * x + y;
    }
};

void saxpy(const float & a, const thrust::device_vector<float> & x, thrust::device_vector<fl
    thrust::transform(x.begin(), x.end(), y.begin(), y.begin(), saxpy_functor(a));
}
```

```
Bandwidth: 15.7344GB/s
Throughput: 7.86722GFlops/s
```

Further Information

- GitHub repository at https://github.com/thrust/thrust
- Documentation at https://thrust.github.io
- Legion scaffold at https://github.com/UCL-RITS/Legion-Fabric-Scaffold/blob/gpu/src/cuda_main.cu
- Tutorial at http://docs.nvidia.com/cuda/thrust/

CUDA-C

CUDA-C Programming Language

- Programming language to write our own GPU kernels
  - based on C99 with extensions
- Compiled with `nvcc`, Nvidia's compiler for CUDA-C
  - comes with Nvidia CUDA Toolkit

- Contains CPU runtime library with functions to
  - transfer data to/from GPU
  - launch “kernel” functions

Kernel functions

- Defined with `__global__` function attribute
  - run multiple times in parallel on the GPU
  - must return `void`
- Callable from CPU code

CUDA Function attributes

- CUDA attributes appear at the start of a function or variable declaration
- `__device__` functions can only be called from other `__device__` functions or `__global__` functions
  - only GPU code is generated
- `__host__` functions can only be called from other `__host__` functions
  - only CPU code is generated
  - optional modifier
  - can be combined with `__device__` to generate code for both CPU and GPU
- `__global__` specifies a function that is called from host code but executed on the GPU
  - must return `void`
  - special calling syntax to specify number of threads, blocks and shared memory

CUDA Data attributes

- `__device__` can also be used to specify a variable that resides in global GPU memory
- `__const__` variables are `const` and are stored in GPU constant memory
  - they can be accessed directly by the host
- `__shared__` variables are stored in shared memory
  - one per block

Variables for thread indexing

- Within GPU code the following variables are defined and read-only:
  - `gridDim` gives the size of the grid
  - `blockIdx` gives the index of the current block in the grid
  - `blockDim` gives the size of the thread blocks
  - `threadIdx` gives the index of the current thread in the block
- These are structs, with e.g. `threadIdx.x` for the x-coordinate.

Calling CUDA

```
saxpy<<<n/64 + 1, 64>>>(n, a, dx, incx, dy, incy);
```

The syntax gives first the gridDim, then the blockDim.

When given as integers, 1-D is assumed.

Otherwise, allocate a `dim3`:

```
dim3 block_dim(32,32,1);
dim3 grid_dim(64,1,1);
kernel<<<grid_dim,block_dim>>>(...);
```

CUDA SAXPY

- The following code snippet implements `saxpy` in CUDA-C:

```
__global__ void saxpy(int n, float a, const float * __restrict__ x, int incx,
                      float * __restrict__ y, int incy) {
    const int i = blockIdx.x * blockDim.x + threadIdx.x;
    if (i < n)
        y[i] += a * x[i];
}
```

```
n = 10000, incx = 1, incy = 1
saxpy: 0.010384ms
```

CUDA SGEMM

- See github.com/garymacindoe/cuda-cholesky for a CUDA SGEMM optimised for older GPUs

```
m = 320, n = 640, k = 640
Bandwidth: 113.432GB/s
Throughput: 28.358GFlops/s
```

More on CUDA

- NVidia CUDA tutorial
- NVidia CUDA Developer Zone
- Legion Scaffold

Another CUDA Example

Monte Carlo PI

- There's a very slow way to calculate π using a fair random number generator.
- Consider throwing darts at a square wall with a dartboard in the middle.
- Your darts are evenly distributed inside the square of side $2r$
- The chance of a dart hitting the dartboard is $\pi r^2/4r^2 = \pi/4$

Monte Carlo Pi

- On each core, generate a random x- and y- coordinate in $[0, 1)$
- Sum-square them, determine if < 1
- Reduce on mean
- Result is pi

CUDA with MPI

- The Emerald supercomputer has a GPU on every node.
- So we can use MPI with CUDA
- The world's fastest computers use accelerators in conjuction with MPI

Let's implement this using CUDA and thrust.

- See GitHub

OpenCL

Why OpenCL?

CUDA only works on NVidia cards.

OpenCL is an open standard which works on all graphics cards, and also on FPGAs.

It uses similar models - copying memory from device to host, launch of kernels with specified thread count and block size. Block size is called "work group size" in OpenCL. (Roughly)

Why not OpenCL

However, there is no equivalent of the Thrust C++ library, and OpenCL kernels may only include C code. (This should change with OpenCL 2.0, but hardware support for this is poor.)

Further, compilation of OpenCL code requires the use of a cumbersome C interface to dispatch source code for compilation and linkage.

OpenCL example

See Legion Scaffold.

Chapter 11

Cloud computing and big data

Cloud computing and big data

Big data

Some data requires special treatment for collection, storage, and analysis.

The ‘three vs’:

- volume
- velocity
- variety

Cloud computing

Cloud computing is an approach built around the concept of shared resources.

- dynamically add and remove computing resources as you need them.
- bring up large clusters of computing power, then shut it own just as quickly

X* as a service

Emergence of service oriented approaches:

- Platform as a service (PaaS)
- Software as a service (SaaS)
- Infrastructure as a service (SaaS)

Exercise 1: Working in the cloud

Spinning up an instance

This example briefly run through the process of:

- creating an account with a provider of cloud services
- spinning up a single cloud instance using a web interface

Create an account

A growing number of companies are offering cloud computing services, for example:

- Amazon Web Services: http://aws.amazon.com
- Cloudera: http://www.rackspace.co.uk/cloud
- Google Cloud Platform: https://cloud.google.com
- Microsoft Azure: http://azure.microsoft.com

Create a key pair

In this exercise we will be working with Amazon Web Services.

Amazon uses public key cryptography to authenticate users, so we'll need to create a private/public key pair:

```
# Create a key pair
$ ssh-keygen -t rsa -f ~/.ssh/ec2 -b 4096
```

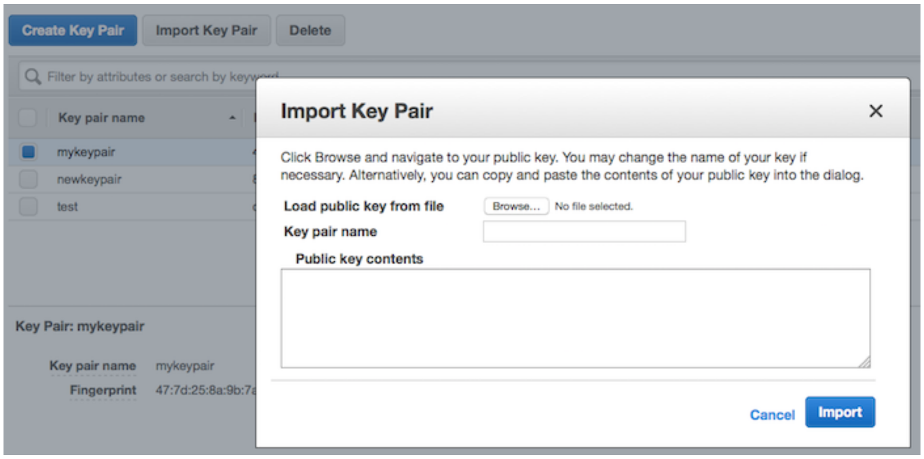
We then need to register our public key with Amazon Web Services.

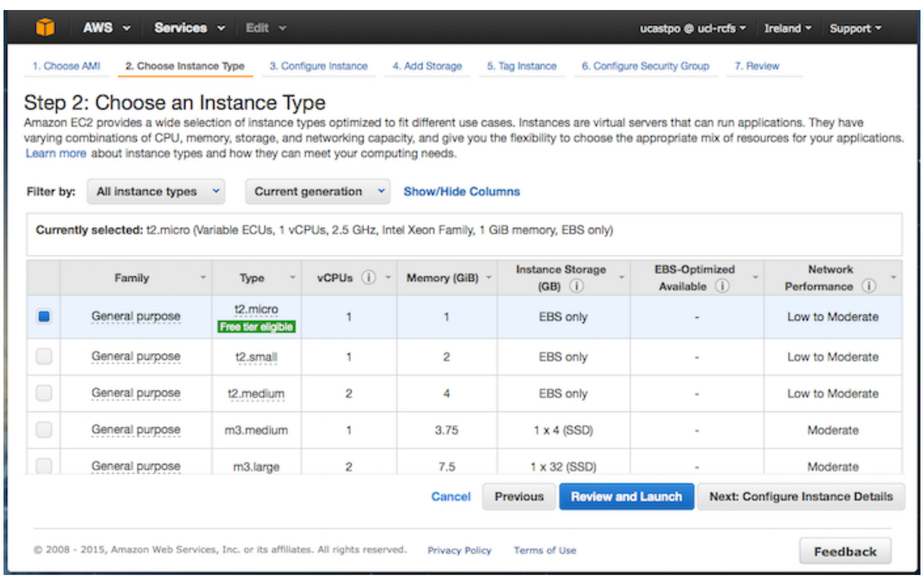
Create a single instance using the web interface

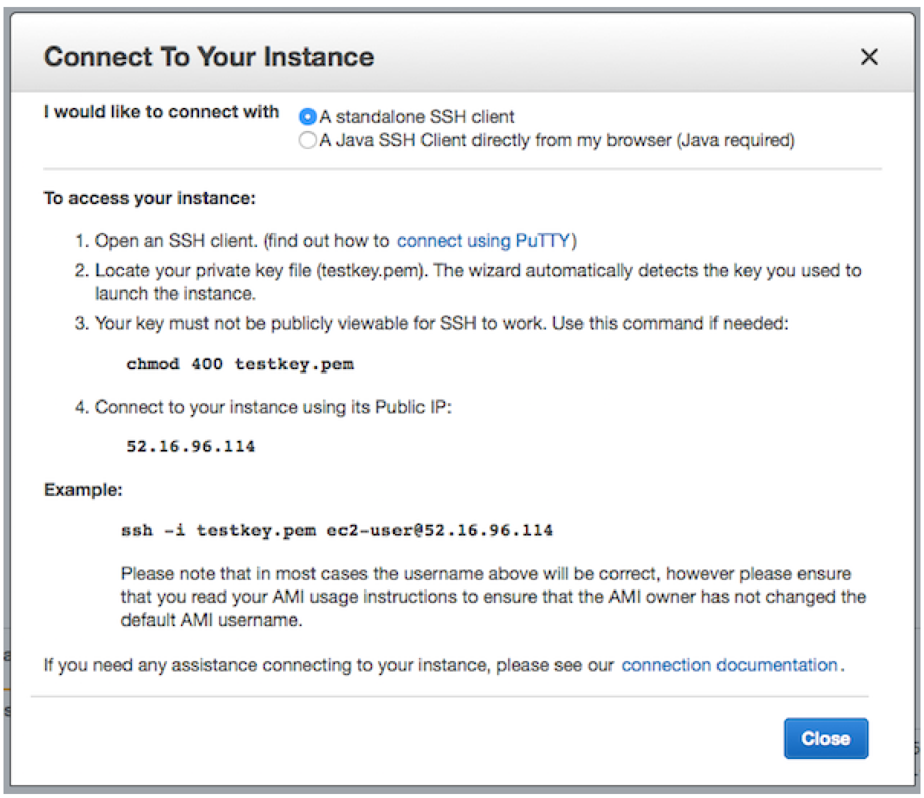
Navigate to the EC2 Dashboard and create a 'micro' instance (1 CPU, 2.5GHZ, 1GB RAM):

Connect to the instance with SSH

For Linux instances, the username is 'ec2-user':


Create Key Pair
Import Key Pair
Delete
Key pair name
mykeypair
newkeypair
test
Key Pair: mykeypair
Key pair name mykeypair
Fingerprint 47:7d:25:8a:9b:7
Import Key Pair
Click Browse and navigate to your public key. You may change the name of your key if necessary. Alternatively, you can copy and paste the contents of your public key into the dialog.
Load public key from file
Browse...
No file selected.
Key pair name
Public key contents
Cancel
Import


AWS
Services
Edit
ucastpo @ ucl-rcfs
Ireland
Support
1. Choose AMI
2. Choose Instance Type
3. Configure Instance
4. Add Storage
5. Tag Instance
6. Configure Security Group
7. Review
Step 2: Choose an Instance Type
Amazon EC2 provides a wide selection of instance types optimized to fit different use cases. Instances are virtual servers that can run applications. They have varying combinations of CPU, memory, storage, and networking capacity, and give you the flexibility to choose the appropriate mix of resources for your applications. Learn more about instance types and how they can meet your computing needs.
Filter by:
All instance types
Current generation
Show/Hide Columns
Currently selected: t2.micro (Variable ECUs, 1 vCPUs, 2.5 GHz, Intel Xeon Family, 1 GiB memory, EBS only)
Family
Type
vCPUs
Memory (GiB)
Instance Storage (GB)
EBS-Optimized Available
Network Performance
General purpose
t2.micro
Free tier eligible
1
1
EBS only
-
Low to Moderate
General purpose
t2.small
1
2
EBS only
-
Low to Moderate
General purpose
t2.medium
2
4
EBS only
-
Low to Moderate
General purpose
m3.medium
1
3.75
1 x 4 (SSD)
-
Moderate
General purpose
m3.large
2
7.5
1 x 32 (SSD)
-
Moderate
Cancel
Previous
Review and Launch
Next: Configure Instance Details
© 2008 - 2015, Amazon Web Services, Inc. or its affiliates. All rights reserved.
Privacy Policy
Terms of Use
Feedback


Connect To Your Instance
I would like to connect with
A standalone SSH client
A Java SSH Client directly from my browser (Java required)
To access your instance:
1. Open an SSH client. (find out how to connect using PuTTY)
2. Locate your private key file (testkey.pem). The wizard automatically detects the key you used to launch the instance.
3. Your key must not be publicly viewable for SSH to work. Use this command if needed:
chmod 400 testkey.pem
4. Connect to your instance using its Public IP:
52.16.96.114
Example:
ssh -i testkey.pem ec2-user@52.16.96.114
Please note that in most cases the username above will be correct, however please ensure that you read your AMI usage instructions to ensure that the AMI owner has not changed the default AMI username.
If you need any assistance connecting to your instance, please see our connection documentation.
Close

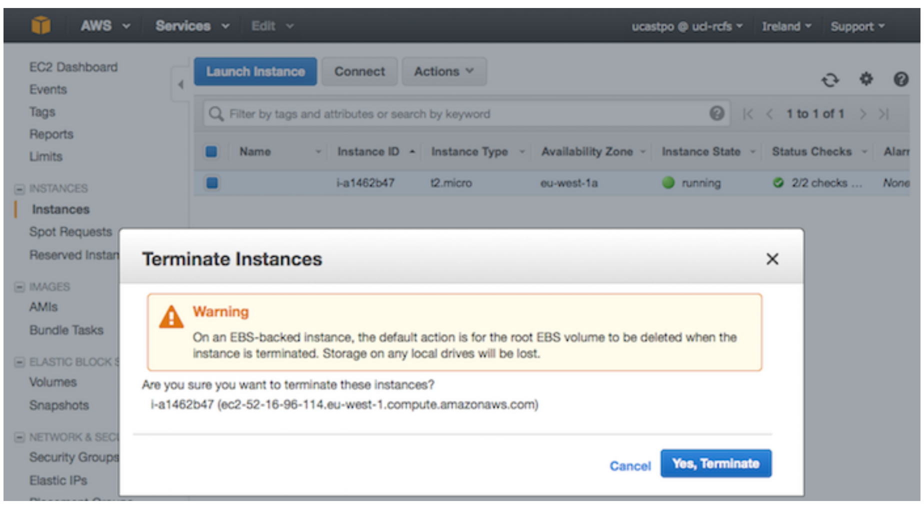
```
# <key_file>: ~/.ssh/ec2
# <public_ID>: 52.16.106.209
$ ssh ec2-user@<public_ID> -i <key_file>


# Connected
       __|  __|_  )
       _|  \(     /   Amazon Linux AMI
      ___|\\___|___|

[ec2-user@ip-xxx ~]$
```

Terminate the server

When finished with the instance, remember to terminate it!



Exercise 2: Working in the cloud

Again, from the command line…

Install Amazon Web Services Command Line Interface:
http://docs.aws.amazon.com/cli/latest/userguide/installing.html

```
# install the tools with pip
sudo pip install awscli
aws ec2 help
```

Configure the tools

To use the command line tools, you'll need to configure your AWS Access Keys, region, and output format:
http://docs.aws.amazon.com/cli/latest/userguide/cli-chap-getting-started.html

```
$ aws configure

# This configuration is stored locally in a home folder named .aws
# On Unix systems: ~/.aws/config;
# On Windows: %UserProfile%\.aws\config
AWS Access Key ID [****************VDLA]: EXXXXXAMPLE
AWS Secret Access Key [****************pa8o]: EXXXXXAMPLE
Default region name [eu-west-1]: eu-west-1
Default output format [json]: json
```

Test our connection to Amazon Web Services

If our connection has been set up correctly, 'describe-regions' will return a list of Amazon Web Service regions:

```
# Successful connection will return list of AWS regions
# HTTPSConnectionPool error? Try changing region to eu-west-1
$ aws ec2 describe-regions
```

Create a key pair

To connect to the instance, we will need a key pair. If you haven't already done so, create one now:

```
# Create an SSH key pair
$ ssh-keygen -t rsa -f ~/.ssh/ec2 -b 4096
```

Transfer the public key to AWS:

```
# <key_name> is a unique name for the pair (e.g. my-key)
# <key_blob> is the public key: "$(cat ~/.ssh/ec2.pub)"
$ aws ec2 import-key-pair --key-name <key_name> \
  --public-key-material <key_blob>
```

Create a security group

We'll also need to create a security group...

```
# creates security group named my-security-group
$ aws ec2 create-security-group \
  --group-name "My security group" \
  --description "SSH access from my local IP address"
```

Configure the security group

...and allow inbound connections from our local IP address:

```
# create a rule to allow inbound connections on TCP port 22
# find your IP: curl http://checkip.amazonaws.com/
$ aws ec2 authorize-security-group-ingress \
  --group-name "My security group" \
  --cidr <local_IP_address>/32 \
  --port 22 \
  --protocol tcp
```

Note: the /32 at the end of the IP address is the bit number of the CIDR netmask. The /32 mask is equivalent to 255.255.255.255, so defines a single host. Lower values broaden the range of allowed addresses. An IP of 0.0.0.0/0 would allow all inbound connections.

Locate an appropriate Machine Image

An Amazon Machine Image contains the software configuration (operating system, software...) needed to launch an instance. AMIs are provided by:

- Amazon Web Services
- the user community
- AWS Marketplace

We will search for an Amazon Machine Image ID (AMI-ID) using the command line tools:

```
# Use filter to locate a specific machine (ami-9d23aeea)
# Filter is a key,value pair
$ aws ec2 describe-images --owners amazon \
  --filters "Name=name,Values=amzn-ami-hvm-2014.09.2.x86_64-ebs"
```

Launch an instance

Launch an instance using the Amazon Machine Image ID:

```
# <AMI-ID>: ami-9d23aeea
# <key_name>: defined when transferring the key
# <group_name>: "My security group"
$ aws ec2 run-instances --image-id <AMI-ID> \
  --key-name <key_name> \
  --instance-type t2.micro \
  --security-groups <group_name>
```

View the instance

We can check the instance and find the public IP:

```
# View information about the EC2 instances
# e.g. state, root volume, IP address, public DNS name
$ aws ec2 describe-instances
```

Connect to the instance

Use the public IP to connect:

```
# for Linux instances, the username is ec2-user
# <public_IP>: 52.16.106.209
# <key_file>: ~/.ssh/ec2
$ ssh -i <key_file> ec2-user@<public_IP>
```

You should now be connected!:

```
# Connected
       __|  __|_  )
       _| \(     /   Amazon Linux AMI
      ___|\\___|___|

[ec2-user@ip-172-31-5-39 ~]$
```

Terminate the instance

Don't forget to terminate the instance when you have finished:

```
# terminate the instance
# <InstanceId>: i-87086760
$ aws ec2 terminate-instances --instance-ids <InstanceId>

TERMINATINGINSTANCES    i-87086760
CURRENTSTATE    32  shutting-down
PREVIOUSSTATE   16  running
```

Virtualisation

Reproducible research

The ability to reproduce the analyses of research studies is increasingly recognised as important.

Several approaches have developed that help researchers to package up code so that their code and dependencies can be distributed and run by others.

Virtual machines

A popular method for creating a shareable environment is with the use of virtual machines.

The isolated system created by virtual machines can be beneficial, but criticisms include:

- size: virtual machines can be bulky
- performance: virtual machines may use significant system resources

Tools such as Vagrant have helped to simplify the process of creating and using virtual machines:
https://www.vagrantup.com

Virtual environments

Virtual environments offer an alternative to virtual machines. Rather than constructing an entirely new system, virtual environments in general seek to provide reproducible 'containers' which are layered on top of an existing environment.

A popular tool for creating virtual environments is Docker:
https://www.docker.com

Exercise 3: Virtualisation

Reproducible research

In this example, we spin up a single EC2 instance and reproduce the analysis from a study in a virtual environment.

The simple analysis uses `countwords`, a shell script, to count the occurrences of words in a book (in our case `dorian.txt`, The Picture of Dorian Gray).

We will be using Docker to manage our virtual environment: https://docs.docker.com/userguide/dockerimages/

Create a new security group

For this exercise we will be setting up a web connection to the EC2 instance, allowing us to connect to IPython Notebook in a browser. To enable this connection, we will create a new security group:

```
$ aws ec2 create-security-group --group-name "ipython_notebook" \
    --description "web access to ipython notebook"
```

We then need to configure this group to allow inbound connections:

```
# SSH
$ aws ec2 authorize-security-group-ingress \
  --group-name "ipython_notebook" \
  --cidr 0.0.0.0/0 \
  --port 22 \
  --protocol tcp
# port 8888
aws ec2 authorize-security-group-ingress \
  --group-name "ipython_notebook" \
  --cidr 0.0.0.0/0 \
  --port 8888 \
  --protocol tcp
```

Spin up a cloud instance

As before, we will now spin up a new cloud instance:

```
# <AMI-ID>: e.g. ami-9d23aeea
# <key_name>: e.g. "my_key"
```

```
# <group_name>: e.g. "ipython_notebook"
$ aws ec2 run-instances --image-id <AMI-ID> \
  --key-name <key_name> \
  --instance-type t2.micro \
  --security-groups <group_name>
```

Connect with SSH

When the instance is running, a public IP will be available:

```
$ aws ec2 describe-instances

"NetworkInterfaces": [
    {
    ...
    "Association": {
        "PublicIp": "12.34.56.78",
        "PublicDnsName": "ec2-12-34-56-78.eu-west-1.compute.amazonaws.com"
     }
     }]
```

Use the public IP to connect over SSH:

```
# <key_file>: e.g. ~/.ssh/ec2
$ ssh ec2-user@<public_IP> -i <key_file>
```

Install and run Docker on the remote system

Docker needs to be installed on the Cloud instance:

```
[ec2-user@ip-xxx ~]$ sudo yum install -y docker
[ec2-user@ip-xxx ~]$ sudo service docker start
```

Docker environments are created by a set of commands

Docker environments are created by running a set of commands held within a Dockerfile. A snippet of the Dockerfile used to create our environment is shown below:

```
# Set the source image
FROM ipython/scipystack:master
```

```
# Specify commands to run inside the image
RUN apt-get update
RUN apt-get install -y wget

# Create directory for container
RUN mkdir /analysis

# Get the code
ADD https://raw.githubusercontent.com/tompollard/dorian/master/mapper.py \
    ~/analysis/mapper.py

# Run notebook
RUN echo "ipython notebook --ip=0.0.0.0 --port=8888 --no-browser" > /usr/bin/notebook.sh; \
chmod 755 /usr/bin/notebook.sh
CMD /usr/bin/notebook.sh

# Open port to the outside world
EXPOSE 8888
...
```

Pull, build, and run the Docker image

Build and run the docker environment:

```
# NB: sudo is not needed when running inside boot2docker
[ec2-user@ip-xxx ~]$ sudo docker pull tompollard/dorian:master
[ec2-user@ip-xxx ~]$ sudo docker run -t --rm=true -p 8888:8888 -i \
    tompollard/dorian:master
```

IPython Notebook is now running in the virtual environment and available to the outside environment on port 8888:

```
[NotebookApp] Using existing profile dir: '/root/.ipython/profile_default'
[NotebookApp] Serving notebooks from local directory: /analysis
[NotebookApp] The IPython Notebook is running at: http://0.0.0.0:8888/
[NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip cor
...
```

Connect to the IPython Notebook

We can now connect to the IPython Notebook in a browser at the public IP of the Amazon Instance on port 8888 (i.e. http://{publicIP}:8888):

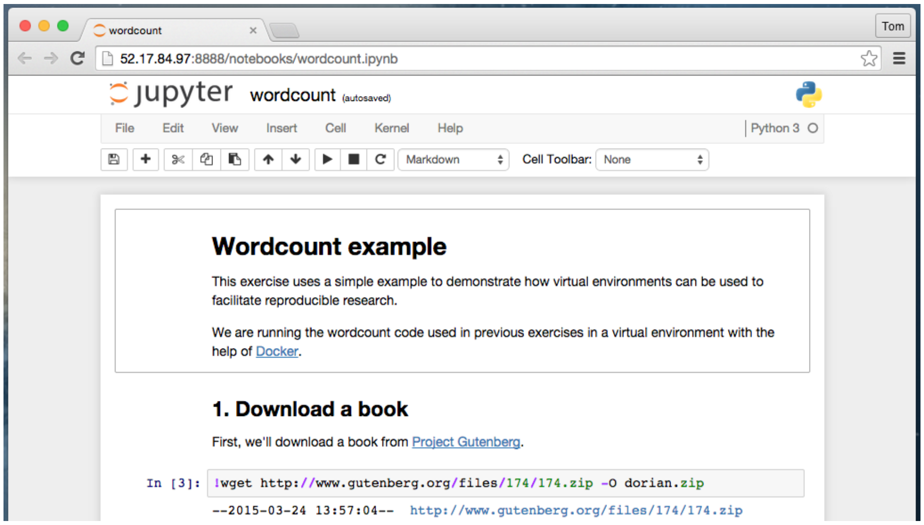


Figure 11.1: IPython Notebook

Now use the IPython Notebook to complete the exercise

Using the IPython Notebook, we can reproduce the analysis on both existing and new datasets.

Distributed computing

Distributed computing

Dividing a problem into many tasks means analysis can be shared across multiple computers, in a parallel fashion.

Cloud computing systems have made distributed computing increasingly accessible to individual users.

Introduced by Google in 2004, MapReduce is a popular model that supports distributed computing on large data sets across clusters of computers.

MapReduce

MapReduce systems are built around the concepts of:

- a mapper, in which the master node takes an input, separates it into sub-problems, and distributes those to worker notes

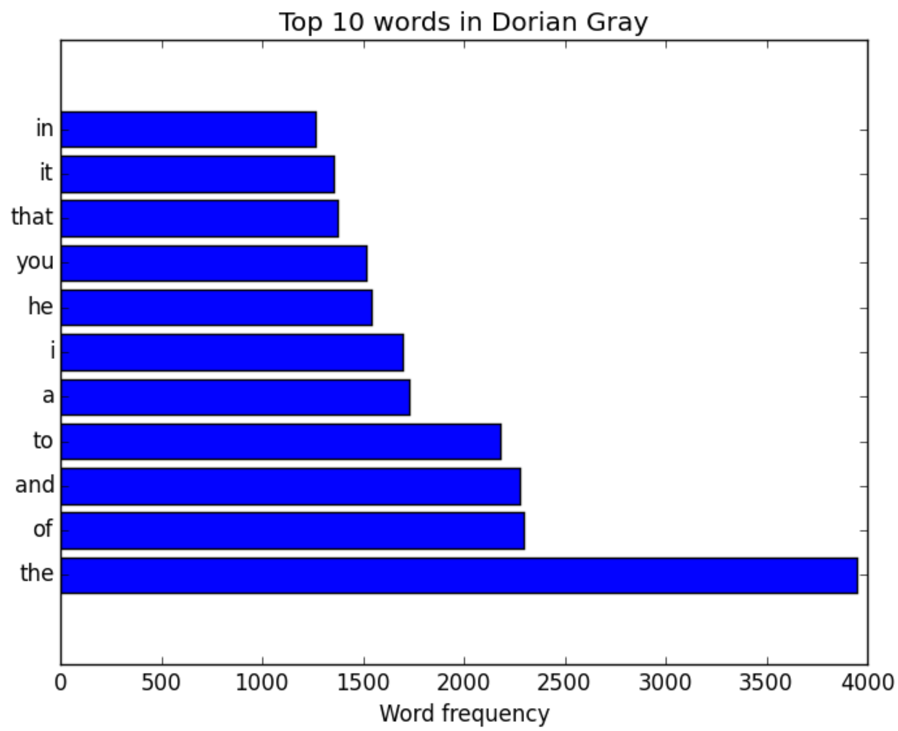


Figure 11.2: Common words in Dorian Gray

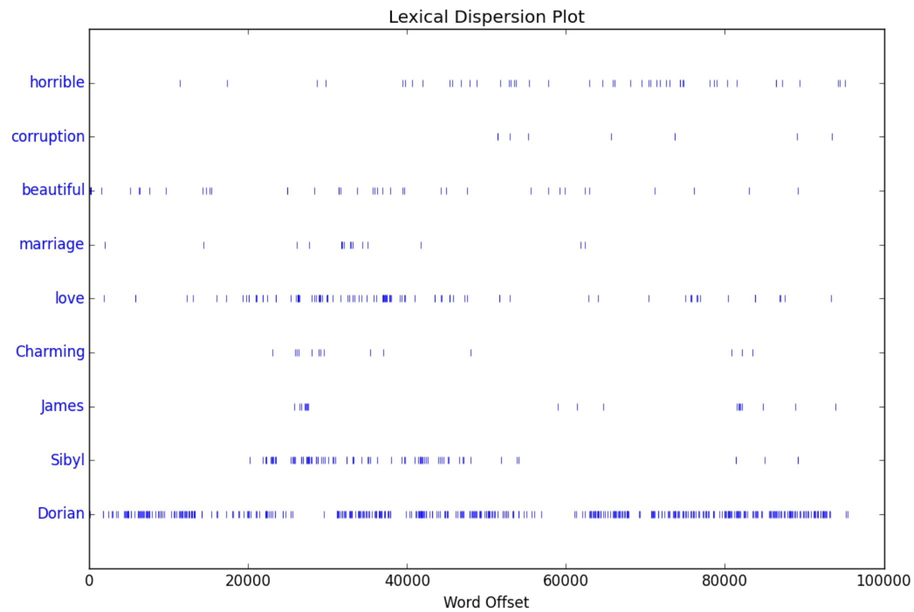


Figure 11.3: Word dispersion

- a 'shuffle' step to distribute data from the mapper
- a reducer which collates the answers to the sub-problems and combines them to solves the initial question.

Distributed file systems

Distributed file systems

- developed to provide reliable data storage across distributed systems
- replicates data across multiple hosts to achieve reliability

Hadoop

Apache Hadoop:

- framework for distributed processing of large data sets
- scales from single servers to many machines
- includes Hadoop MapReduce and the Hadoop Distributed File System

Exercise 4: MapReduce

The 'Hello World' of MapReduce

In this example, we will demonstrate how the mapper and reducer can be applied on our local machines to count the number of times each word appears in a book.

Choose a book

Find a good book on Project Gutenberg and download it: http://www.gutenberg.org/browse/scores/top

```
# The Picture of Dorian Gray
$ wget http://www.gutenberg.org/cache/epub/174/pg174.txt -O dorian.txt
```

```
$ head dorian.txt
```

```
Title: The Picture of Dorian Gray

The artist is the creator of beautiful things.  To reveal art and
conceal the artist is art\'s aim.  The critic is he who can translate
into another manner or a new material his impression of beautiful
things.
```

Hadoop streaming

Hadoop streaming enables MapReduce jobs to be run using any executable as the mapper and reducer: http://hadoop.apache.org/docs/r1.2.1/streaming.html

The mapper and reducer are written to take line-by-line inputs from stdin and emit the output to stdout.

Mapper

Our mapper:

- takes lines from our book
- extracts words from the line with a regular expression
- outputs a tab-separated string,value pair for each word (e.g. theword 1)

```python
#!/usr/bin/env python
import sys
import re

def mapper(stream):
    pattern = re.compile('[a-zA-Z][a-zA-Z0-9]*')
    for line in stream:
        for word in pattern.findall(line):
            print word.lower() + '\t' + '1'

mapper(sys.stdin)
```

Reducer

Our reducer:

- takes the word, value pairs generated by the mapper
- sums the count for each word
- outputs a word, count pair

```python
#!/usr/bin/env python
import sys

def reducer(stream):
    mydict = {}
    line = stream.readline()
    while line:

        # Get the key/value pair
        line = line.strip()
        word, count = line.split('\t')
        count = int(count)

        # Add to the dict
        if word in mydict:
            mydict[word] += 1
        else:
            mydict[word] = 1

        # Get the next line
        line = stream.readline()
```

```
    # Print the aggregated key/value pairs
    # for word in sorted(mydict.keys()): # order by word
    for word in sorted(mydict, key=mydict.get, reverse=True): # or by count
        print word, '\t', mydict[word]

reducer(sys.stdin)
```

Demonstrate locally

Download the mapper and reducer:

```
$ git clone https://github.com/tompollard/dorian
```

Create a pipeline to process the book:

```
# sort represents the Hadoop shuffle
$ cat dorian.txt | ./mapper.py | sort | ./reducer.py | more

the     3948
of      2298
and     2279
to      2181
a       1730
i       1694
he      1544
...
```

Exercise 5: Distributed computing

Again, with Hadoop

In the previous exercise, we demonstrated MapReduce on our local computer.

In this exercise we will spin up multiple cloud instances, making use of Hadoop to carry out a distributed MapReduce operation.

We could set up multiple instances in the cloud (for example with EC2), then configure Hadoop to run across the instances. This is not trivial and takes time.

Hadoop in the cloud

Fortunately, several cloud providers offer configurable Hadoop services. One such service is Amazon Elastic MapReduce (EMR).

Elastic MapReduce provides a framework for:

- uploading data and code to the Simple Storage Service (S3)
- analysing with a multi-instance cluster on the Elastic Compute Cloud (EC2)

Create an S3 bucket

Create an S3 bucket to hold the input data and our map/reduce functions:

1. Open the Amazon Web Services Console: http://aws.amazon.com
2. Select "Create Bucket" and enter a globally unique name
3. Ensure the S3 Bucket shares the same region as other instances in your cluster

Or, through the command line interface:

```
$ aws s3 mb s3://ucl-jh-books-example
```

Copy data and code to S3

Sample map and reduce functions are available on GitHub:

```
# clone the code from a remote repository
$ git clone https://github.com/tompollard/dorian
```

Copy the data and code to S3:

```
# Copy input code and data to S3
# No support for unix-style wildcards
$ aws s3 cp dorian.txt s3://my-bucket-ucl123/input/
$ aws s3 cp mapper.py s3://my-bucket-ucl123/code/
$ aws s3 cp reducer.py s3://my-bucket-ucl123/code/
```

Launch the compute cluster

Create a compute cluster with one master instance and two core instances:

```
# Start a EMR cluster
# <ami-version>: version of the machine image to use
# <instance-type>:  number and type of Amazon EC2 instances
# <key_name>: "mykeypair"
$ aws emr create-cluster --ami-version 3.1.0 \
```

```
    --ec2-attributes KeyName=<key_name> \
    --instance-groups InstanceGroupType=MASTER,InstanceCount=1,InstanceType=m3.xlarge \
    InstanceGroupType=CORE,InstanceCount=2,InstanceType=m3.xlarge

"ClusterId": "j-3HGKJHEND0DX8"
```

Get the cluster ID

Get the cluster-id:

```
# Get the cluster-id
$ aws emr list-clusters
    ...
    "Id": "j-3HGKJHEND0DX8",
    "Name": "Development Cluster"
```

Get the public DNS name of the cluster

When the cluster is up and running, get the public DNS name:

```
# Get the DNS
$ aws emr describe-cluster --cluster-id j-3HGKJHEND0DX8 \
    | grep MasterPublicDnsName
    ...
    "MasterPublicDnsName": "ec2-52-16-235-144.eu-west-1.compute.amazonaws.com"
```

Connect to the cluster

SSH into the cluster using the username 'hadoop':

```
# SSH into the master node
# <key_file>: ~/.ssh/ec2
# <MasterPublicDnsName>: ec2-52-16-235-144.eu-west-1.compute.amazonaws.com
$ ssh hadoop@<MasterPublicDnsName> -i <key_file>

# Connected
       __|  __|_  )
       _| \(     /   Amazon Linux AMI
      ___|\\___|___|

[hadoop@ip-xxx ~]$
```

Run the analysis

```
# To process multiple input files, use a wildcard
[hadoop@ip-xxx ~]$ hadoop \
    jar contrib/streaming/hadoop-*streaming*.jar \
    -files s3://my-bucket-ucl123/code/mapper.py,s3://my-bucket-ucl123/code/reducer.py \
    -input s3://my-bucket-ucl123/input/* \
    -output s3://my-bucket-ucl123/output/ \
    -mapper mapper.py \
    -reducer reducer.py
```

View the results

Results are saved to the output folder. Each reduce task writes its output to a separate file:

```
# List files in the output folder
$ aws s3 ls s3://my-bucket-ucl123/output/
```

Download the output:

```
# Copy the output files to our local folder
# No support for unix-style wildcards, so use --recursive
$ aws s3 cp s3://my-bucket-ucl123/output . --recursive

# View the file
$ head part-00001
```

```
the     3948
and     2279
in      1266
his     996
lord    248
...
```

Terminate the cluster

Once our analysis is complete, terminate the cluster:

```
# get cluster id: aws emr list-clusters
# <cluster_ID>: j-3HGKJHEND0DX8
$ aws emr terminate-clusters --cluster-id <cluster_ID>
```

Delete the bucket

```
$ aws s3 rb s3://my-bucket-ucl123 --force
```

Chapter 12

Appendix - Template Meta-Programming

Appendix - Template Meta-Programming

No Longer In Course

- Notes provided here for historical reasons.
- Also, read "Modern C++ Design"

Template Meta-Programming (TMP)

What Is It?

- See Wikipedia, Wikibooks, Keith Schwarz
- C++ Template
  - Type or function, parameterised over, set of types, constants or functions
  - Instantiated at compile time
- Meta Programme
  - Program that produces or manipulates constructs of target language
  - Typically, it generates code
- Template Meta-Programme
  - C++ programme, uses Templates, generate C++ code at compile time

TMP is Turing Complete

- Given: A Turing Machine
  - Tape, head, states, program, etc.
- A language is "Turing Complete" if it can simulate a Turing Machine
  - e.g. Conditional branching, infinite looping
- Turing's work underpins much of "what can be computed" on a modern computer
  - C, C++ no templates, C++ with templates, C++ TMP
  - All Turing Complete
- Interesting that compiler can generate such theoretically powerful code.
- But when, where, why, how to use TMP?
- (side-note: Its not just a C++ pre-processor macro)

Why Use It?

- Use sparingly as code difficult to follow
- Use for
  - Optimisations
  - Represent Behaviour as a Type
  - Traits classes
- But when you see it, you need to understand it!

Factorial Example

See Wikipedia Factorial Example

- This:

```
#include <iostream>
using namespace std;

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

```
template <>
struct factorial<0> {
    enum { value = 1 };
};

int main () {
  std::cout << factorial<0>::value << std::endl;
  std::cout << factorial<8>::value << std::endl;
}
```

- Produces:

```
1
40320
```

Factorial Notes:

- Compiler must know values at compile time
  - i.e. constant literal or constant expression
  - See also constexpr
- Generates/Instantiates all functions recursively
- Factorial 16 = 2004189184
- Factorial 17 overflows
- This simple example to illustrate "computation"
- But when is TMP actually useful?
- Notice that parameter was an integer value ... not just "int" type

Loop Example

- This:

```
#include <iostream>
#include <vector>
using namespace std;

template<typename T>
T Sum(const std::vector<T>& data)
{
  T total = 0;
  for (size_t i = 0; i < data.size(); i++)
  {
    total += data[i];
```

```
  }
  return total;
}

int main () {
  size_t numberOfInts = 3;
  size_t numberOfLoops = 1000000000;
  vector<int> a(numberOfInts);
  int total = 0;

  std::cout << "Started" << std::endl;
  for (size_t j = 0; j < numberOfLoops; j++)
  {
    for (size_t i = 0; i < numberOfInts; i++)
    {
      total = Sum(a);
    }
  }
  std::cout << "Finished:" << total << std::endl;
}
```

- Time: numberOfInts=3 took 40 seconds

Loop Unrolled

- This:

```
#include <iostream>
#include <vector>
using namespace std;

template <typename T, int length>
class FixedVector {
   T data[length];
  public:
    FixedVector()
    {
      // Initialise
      for (size_t i = 0; i < length; i++)
      {
        data[i] = 0;
      }
    }
    T Sum()
```

```
    {
      T sum = 0;
      for (size_t i = 0; i < length; i++)
      {
        sum += data[i];
      }
      return sum;
    }
};

int main () {
  const size_t numberOfInts = 3;
  const size_t numberOfLoops = 1000000000;
  FixedVector<int, numberOfInts> a;
  int total = 0;

  std::cout << "Started" << std::endl;
  for (size_t j = 0; j < numberOfLoops; j++)
  {
    for (size_t i = 0; i < numberOfInts; i++)
    {
      total = a.Sum();
    }
  }
  std::cout << "Finished:" << total << std::endl;
}
```

- Time: numberOfInts=3 took 32 seconds when switch to fixed vector, and 23 when a raw array.

Policy Checking

- Templates parameterised by type not by behaviour
- But you can make a class to represent the behaviour
- See Keith Schwarz for longer example.

Simple Policy Checking Example

- This:

```
#include <iostream>
#include <vector>
#include <stdexcept>
```

```
class NoRangeCheckingPolicy {
  public:
    static void CheckRange(size_t pos, size_t n) { return; } // no checking
};

class ThrowErrorRangeCheckingPolicy {
  public:
    static void CheckRange(size_t pos, size_t n)
    {
      if (pos >= n) { throw std::runtime_error("Out of range!"); }
    }
};

template < typename T
         , typename RangeCheckingPolicy = NoRangeCheckingPolicy
         >
class Vector
 : public RangeCheckingPolicy
{

  private:
    std::vector<T> data;
  public:
    // other methods etc.
    const T& operator[] (size_t pos) const
    {
      RangeCheckingPolicy::CheckRange(pos, data.size());
      return data[pos];
    }
};

int main () {
  Vector<int, ThrowErrorRangeCheckingPolicy> a;
  // a.push_back(1); or similar
  // a.push_back(2); or similar
  try {
    std::cout << a[3] << std::endl;
  } catch (const std::runtime_error& e)
  {
    std::cerr << e.what();
  }
  return 0;
}
```

- Produces:

Summary of Policy Checking Example

- Define interface for behaviour
- Parameterize over all behaviours
- Use multiple-inheritance to import policies
- e.g. logging / asserts

Traits

- From C++ standard 17.1.18
  - "a class that encapsulates a set of types and functions necessary for template classes and template functions to manipulate objects of types for which they are instantiated."
- Basically: Traits represent details about a type
- You may be using them already!
- Start with a simple example

Simple Traits Example

- This:

```
#include <iostream>

template <typename T>
struct is_void {
  static const bool value = false;
};

template <>
struct is_void<void> {
  static const bool value = true;
};

int main () {
  std::cout << "is_void(void)=" << is_void<void>::value << std::endl;
  std::cout << "is_void(int)=" << is_void<int>::value << std::endl;
  return 0;
}
```

- Produces:

```
is_void(void)=1
is_void(int)=0
```

Traits Principles

- Small, simple, normally public, eg. struct
- else/if
  - Else template
  - partial specialisations
  - full specialisations
- Probably using them already
  - `std::numeric_limits<double>::max()`
  - ITK has similar `itk::NumericTrait<PixelType>`
- Applies to primatives as well as types

Traits Examples

- Simple Tutorial from Aaron Ballman
- Boost meta-programming support
- Boost type_traits tutorial
- C++11 has many traits

Wait, Inheritance Vs Traits?

- We said inheritance is often overused in OO
- We say that too frequent if/switch statements based on type are bad in OO
- C++11 providing many is_X type traits returning bool, leading to if/else
- So, when to use it?

When to use Traits

- Some advice
  - Sparingly
  - To add information to templated types
  - Get algorithm to work for 1 data type
  - If you extend to multiple data types and consider templates
    - When you need type specific behaviour

- traits probably better than template specialisation
- traits better than inheritance based template hierarchies

- Remember
  - Scientist = few use-cases
  - Library designer = coding for the unknown, and potentially limitless use-cases
    - More likely of interest to library designers

TMP Use in Medical Imaging - 1

Declare an ITK image

```
template< typename TPixel, unsigned int VImageDimension = 2 >
class Image:public ImageBase< VImageDimension >
{
public:
// etc
```

- TPixel, `int`, `float` etc.
- VImageDimension = number of dimensions

TMP Use in Medical Imaging - 2

But what type is origin/spacing/dimensions?

```
template< unsigned int VImageDimension = 2 >
class ImageBase:public DataObject
{
  typedef SpacePrecisionType                             SpacingValueType;
  typedef Vector< SpacingValueType, VImageDimension > SpacingType;
```

TMP Use in Medical Imaging - 3

So now look at `Vector`

```
template< typename T, unsigned int NVectorDimension = 3 >
class Vector:public FixedArray< T, NVectorDimension >
{
public:
```

TMP Use in Medical Imaging - 4

Now we can see how fixed length arrays are used

```
template< typename T, unsigned int TVectorDimension >
const typename Vector< T, TVectorDimension >::Self &
Vector< T, TVectorDimension >
::operator+=(const Self & vec)
{
  for ( unsigned int i = 0; i < TVectorDimension; i++ )
    {
    ( *this )[i] += vec[i];
    }
  return *this;
}
```

which may be unrolled by compiler.

TMP Use in Medical Imaging - 5

- ITK
  - uses `itk::NumericTraits<>` adding mathematical operators like multiplicative identity, additive identity
  - uses traits to describe features of meshes, `like numeric_limits`, but more generalised
- MITK (requires coffee and a quiet room)
  - uses mitkPixelTypeList.h for multi-plexing across templated image to non-templated image type
  - uses mitkGetClassHierarchy.h to extract a list of class names in the inheritance hierarchy
- TMP in B-spline based registration:

Further Reading For Traits

- Keith Schwarz
- Nathan Meyers
- Todd Veldhuizen, traits scientific computing
- Thaddaaeus Frogley, ACCU, traits tutorial
- Aaron Ballman
- Andrei Alexandrescu
- Andrei Alexandrescu traits with state

- Boost meta-mrogramming support
- Boost type_traits tutorial
- C++11 has many traits

Further Reading In General

- Andrei Alexandrescu's Book
- Herb Sutter's Guru of The Week, especially 71 and this article
- And of course, keep reading Meyers

Summary

- Learnt
  - Notation for template function/class/meta-programming
  - Uses and limitations of template function/class
  - Template Meta-Programming
    - Optimisation, loop unrolling
    - Policy classes
    - Traits

Chapter 13

Linux Install

Git

If git is not already available on your machine you can try to install it via your distribution package manager (e.g. `apt-get` or `yum`).

On ubuntu or other Debian systems:

```
sudo apt-get install git
```

On RedHat based systems:

```
sudo yum install git
```

Subversion

Again, install the appropriate package with apt-get or yum (`subversion`)

CMake

Again, install the appropriate package with apt-get or yum (`cmake`)

Editor and shell

Many different text editors suitable for programming are available. If you don't already have a favourite, you could look at Kate.

Regardless of which editor you have chosen you should configure git to use it. Executing something like this in a terminal should work:

```
git config --global core.editor NameofYourEditorHere
```

The default shell is usually bash but if not you can get to bash by opening a terminal and typing `bash`.

Chapter 14

Windows Install

Git

Install msysgit

Then install the GitHub for Windows client.

Subversion

Install subversion

And choose to add it to the path for all users if so prompted.

CMake

Install cmake

And choose to add it to the path for all users if so prompted.

Editor

Unless you already use a specific editor which you are comfortable with we recommend using *Notepad++* on windows.

Using Notepad++ to edit text files including code should be straight forward but in addition you should configure git to use notepad++ when writing commit messages (We will learn about these in the version controle session).

Unix tools

Install MinGW by following the download link. It should install MinGW's package manager. On the left, select `Basic Setup`, and on the right select `mingw32-base`, `mingw-developer-toolkit, mingw-gcc-g++` and `msys-base`. On some systems these package might be selected from start. Finally, click the installation menu and `Apply Changes`.

Locating your install

Now, we need to find out where Git and Notepad++ have been installed, this will be either in `C:/Program Files (x86)` or in `C:\ProgramFiles`. The former is the norm on more modern versions of windows. If you have the older version, replace `Program\ Files\ \(x86\)` with `Program\ Files` in the instructions below.

Telling Shell where to find the tools

We need to tell the new shell installed in this way where git and Notepad++ are.

To do this, use NotePad++ to edit the file at `C:\MinGW\mysys\1.0\etc\profile`

and toward the end, above the line `alias clear=clsb` add the following:

```
# Path settings from SoftwareCarpentry
export PATH=$PATH:/c/Program\ Files\ \(x86\)/Git/bin
export PATH=$PATH:/c/Program\ Files\ \(x86\)/Notepad++
# End of Software carpentry settings
```

Finding your terminal

Check this works by opening MinGW shell, with the start menu (Start->All programs->MinGW->MinGW Shell). This should open a *terminal* window, where commands can be typed in directly.

On windows 8, there may be no app for MinGW. In that case, open the `run` app and type in

```
C:\MinGW\msys\1.0\msys.bat
```

Checking which tools you have

Once you have a terminal open, type

```
which notepad++
```

which should produce readout similar to

```
/c/Program Files (x86)/Notepad++/notepad++.exe`
```

Also try:

```
which git
```

which should produce

```
/c/Program Files (x86)/Notepad++/notepad++.exe
```

The `which` command is used to figure out where a given program is located on disk.

Tell Git about your editor

Now we need to update the default editor used by Git.

```
git config --global core.editor "'C:/Program Files (x86)/Notepad++
    /notepad++.exe' -multiInst  -nosession -noPlugin"
```

Note that it is not obvious how to copy and paste text in a Windows terminal including Git Bash. Copy and paste can be found by right clicking on the top bar of the window and selecting the commands from the drop down menu (in a sub menu).

You should now have a working version of git and notepad++, accessible from your shell.

Chapter 15

Mac Install

XCode and command line tools

Install XCode using the Mac app store.

Then, go to Xcode… Preferences… Downloads… and install the command line tools option

Git

Install Homebrew via typing this at a terminal:

```
ruby -e "$(curl -fsSL https://raw.github.com/mxcl/homebrew/go)"
```

and then type

```
brew install git
```

Then install the GitHub for Mac client. (If you have problems with older versions of OSX, it's safe to skip this.)

CMake

Just do

```
brew install cmake
```

Editor and shell

The default text editor on OS X *textedit* should be sufficient for our use. Alternatively choose from a list of other good editors.

To setup git to use *textedit* executing the following in a terminal should do.

```
git config --global core.editor
    /Applications/TextEdit.app/Contents/MacOS/TextEdit
```

The default terminal on OSX should also be sufficient. If you want a more advanced terminal iTerm2 is an alternative.

Chapter 16

Installing Boost

Linux Users

Install the appropriate package with apt-get or yum, for example:

```
sudo apt-get install boost
```

On Ubuntu 13.04 boost is spilt into multiple packages. The package needed here is “libboost1.53-dev” and to install it you should do:

```
sudo apt-get install libboost1.53-dev
```

Check that your package manager is delivering at least version 1.53, if you have an earlier version, you will need to download from source, following the windows instructions below.

Mac Users

```
brew install boost
```

Windows Users

You will need to download and install boost manually.

Create an appropriate folder, somewhere near your working code for the course.

For example, if you are working in `/home/myusername/devel/cppcourse/rsd-cppcourse/reactor` you could do:

```
mkdir -p ~/devel/libraries/boost
cd ~/devel/libraries/boost
```

Now, download and unzip boost, which will take quite a while:

```
curl -L http://sourceforge.net/projects/boost/files/...
        ...boost/1.54.0/boost_1_54_0.zip/download > boost.zip
unzip boost.zip
```

(All one line, not literally two lines with dots!)

CMake and Boost

If we download from source, before we next build, we will need to tell our shell where the boost library can be found

```
cd build
export CMAKE_INCLUDE_PATH=/home/myusername/devel/libraries/boost_1_54_0
cmake ..
make
ctest
```

... or your equivalent.

Chapter 17

Installation

Installation Instructions

Introduction

This document contains instructions for installation of the packages we'll be using during the course. You will be following the training on your own machines, so please complete these instructions. You don't need everything before lecture one: you can refer to these instructions as the course proceeds.

What you'll need by the end of the course

- CMake build tool.
- Catch unit testing framework.
- Git and the GitHub website.
- Some C++ libraries: The Boost C++ library package, and ITK, the Insight Toolkit
- An SSH Client for remote access with an SSH keypair
- Fabric remote server access scripting library for Python.
- X client
- A code editor of your choice.

Eduroam

We will be using UCL's eduroam service to connect to the internet for this work.

So you should ensure you have eduroam installed and working.

Assignment 2

Serial Solution

Build a C++ implementation of Conway's Game of Life. See for example https://en.wikipedia.org/wiki/Conway%27s_Game_of_Life [5 Marks]

Marks Scheme:

- Valid code: 1 mark.
- Readable code: 1 marks.
- Appropriate unit tests: 1 marks.
- Well-structured project layout and build system: 1 mark.
- Use of version control: 1 mark.

Organising remote computation

Define an appropriate output file format, and use a script in a dynamic language (Python, MATLAB, R, Ruby, Perl etc) to create an mpeg video of your results. Use a script to deploy your serial code on a remote cluster with qsub. [5 marks]

Marks scheme:

- Output file works: 1 mark.
- Visualiser works: 1 mark.
- Automated deployment script with fabric or bash: 1 mark.
- Output file and script organisation support reproducible research: 1 mark.
- Valid job submission script: 1 mark.

Shared memory parallelism

Parallelise your code using OpenMP. Create a graph of performance versus core count on a machine with at least 12 cores. Comment on your findings. [5 Marks]

Marks scheme:

- Valid OpenMP parallelisation: 1 mark.
- Preprocessor usage so that code remains valid without OpenMP: 1 mark
- Script to organise job runs and results for performance measurement: 1 mark.
- Clear and meaningful scaling graph: 1 mark.
- Discussion: 1 mark

Distributed memory parallelism

Parallelise your code using MPI, with a 2-dimensional spatial decomposition scheme. Create a performance graph with at least 12 cores. Comment on your findings. [5 marks]

Marks scheme:

- Valid MPI parallelisation: 1 mark.
- Valid 2-dimensional decomposition scheme: 1 mark.
- Unit tests to exercise decomposition sheme: 1 mark.
- Performance graph, with script to organise measurement runs and clear graph: 1 mark
- Discussion: 1 mark

Accelerators

Accelerate your serial solution using at least one of CUDA Thrust, CUDA C or OpenCL. Experiment with different thread counts and performance optimisations. Measure speedup compared to the serial code, either on a cluster or using a graphics card on your own computer. Comment on your findings. (There is one mark available for a second accelerator solution.) [5 marks]

Marks scheme:

- Valid accelerator parallelisation: 1 mark
- Clean, readable, tested code: 1 mark
- Optimisation by exploring different thread counts and other configurable parameters: 1 mark
- Speedup analysis and discussion: 1 mark
- Second accelerator parallelisation: 1 mark.

Submission of the assignment

You should submit your solution via Moodle, including the entire code repository with version control history. Your solution should include a text report with a discussion of your project and a clear explanation of how to build and invoke your code – the marker will deduct marks if the code cannot easily be built and run as indicated. Your report should be broken down into sections that reflect those of the assignment, and should include your graphs, performance measurements, and discussion of any problems or interesting design decisions you encounter along the way. You should separate your solutions for each section with version control revision numbers, tags or branches and describe these in the report.

Chapter 18

Assessment

Assessment Structure

- 3 hour exam
  - Past papers from 2015 and later are available
  - Past marks schemes and standard solutions are not available
- 2 pieces coursework - 40 hours each
  - 1 due 3rd week March
  - ## 1 due just after Easter

    title: Research Computing with C++ author:

- Matt Clarkson
- James Hetherington
- Mayeul d'Avezac
- ## Jens H Nielsen