

AMATH 483/583 High Performance Scientific Computing

Lecture 2: Variables, functions, parameters

Andrew Lumsdaine
Northwest Institute for Advanced Computing
Pacific Northwest National Laboratory
University of Washington
Seattle, WA

Administrivia

- PS1 to be posted this afternoon
- Sign up for piazza (link on canvas)
- Sign up for course notebook (canvas / onenote)

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Overview

- Recap of Lecture 1
- Types and variables
- Namespaces
- Functions and procedural abstraction
- Parameter passing

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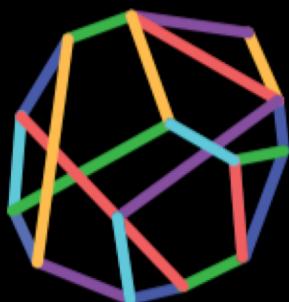
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SC'19 Student Cluster Competition Call-Out!

- Teams work with advisor and vendor to design and build a cutting-edge, commercially available cluster constrained by the 3000-watt power limit
- Cluster run a variety of HPC workflows, ranging from being limited by CPU performance to being memory bandwidth limited to I/O intensive
- Teams are comprised of six undergrad or high-school students plus advisor



SC19

<https://sc19.supercomputing.org/program/studentssc/student-cluster-competition/>

Informational meeting:
Tu 5PM-6PM Allen 203
Th 5PM-6PM Allen 203

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In Our Last Exciting Episode

- “High Performance” = bigger, better, faster, more
 - Use resources as efficiently as possible
 - Starting with single core
 - Use multiple cores/sockets/boards/blades/nodes/racks
- Moore’s law → miniaturization → higher clock rates → performance
 - “Denard scaling” ended c. 2005
- Moore’s law → miniaturization → more transistors → more cores
- Gordon Moore, Seymour Cray, Thomas Sterling
- Top 500 List (top500.org)

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Top 500 November 2017

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	National Supercomputing Center in Wuxi China	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9	15,371
2	National Super Computer Center in Guangzhou China	Tianhe-2 (MilkyWay-2) - TH-IVB-FEP Cluster, Intel Xeon E5-2692 12C 2.200GHz, TH Express-2, Intel Xeon Phi 31S1P NUDT	3,120,000	33,862.7	54,902.4	17,808
3	DOE/SC/Oak Ridge National Laboratory United States	Titan - Cray XK7 , Opteron 6274 16C 2.200GHz, Cray Gemini interconnect, NVIDIA K20x Cray Inc.	560,640	17,590.0	27,112.5	8,209
4	DOE/NNSA/LLNL United States	Sequoia - BlueGene/Q, Power BQC 16C 1.60 GHz, Custom IBM	1,572,864	17,173.2	20,132.7	7,890

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Top500 November 2017

5	DOE/SC/LBNL/NERSC United States	Cori - Cray XC40, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect Cray Inc.	622,336	14,014.7	27,880.7	3,939
6	Joint Center for Advanced High Performance Computing Japan	Oakforest-PACS - PRIMERGY CX1640 M1, Intel Xeon Phi 7250 68C 1.4GHz, Intel Omni-Path Fujitsu	556,104	13,554.6	24,913.5	2,719
7	RIKEN Advanced Institute for Computational Science (AICS) Japan	K computer, SPARC64 VIIIfx 2.0GHz, Tofu interconnect Fujitsu	705,024	10,510.0	11,280.4	12,660
8	Swiss National Supercomputing Centre (CSCS) Switzerland	Piz Daint - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 Cray Inc.	206,720	9,779.0	15,988.0	1,312

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Top500 November 2018

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	DOE/SC/Oak Ridge National Laboratory United States	Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband IBM	2,397,824	143,500.0	200,794.9	9,783
2	DOE/NNSA/LLNL United States	Sierra - IBM Power System S922LC, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband IBM / NVIDIA / Mellanox	1,572,480	94,640.0	125,712.0	7,438
3	National Supercomputing Center in Wuxi China	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway NRCPC	10,649,600	93,014.6	125,435.9	15,371
4	National Super Computer Center in Guangzhou China	Tianhe-2A - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000 NUDT	4,981,760	61,444.5	100,678.7	18,482



1.5M
cores

10M
cores

Top500 November 2018

5	Swiss National Supercomputing Centre (CSCS) Switzerland	Piz Daint - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 Cray Inc.	387,872	21,230.0	27,154.3	2,384
6	DOE/NNSA/LANL/SNL United States	Trinity - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect Cray Inc.	979,072	20,158.7	41,461.2	7,578
7	National Institute of Advanced Industrial Science and Technology (AIST) Japan	AI Bridging Cloud Infrastructure (ABCi) - PRIMERGY CX2570 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR Fujitsu	391,680	19,880.0	32,576.6	1,649
8	Leibniz Rechenzentrum Germany	SuperMUC-NG - ThinkSystem SD530, Xeon Platinum 8174 24C 3.1GHz, Intel Omni-Path Lenovo	305,856	19,476.6	26,873.9	

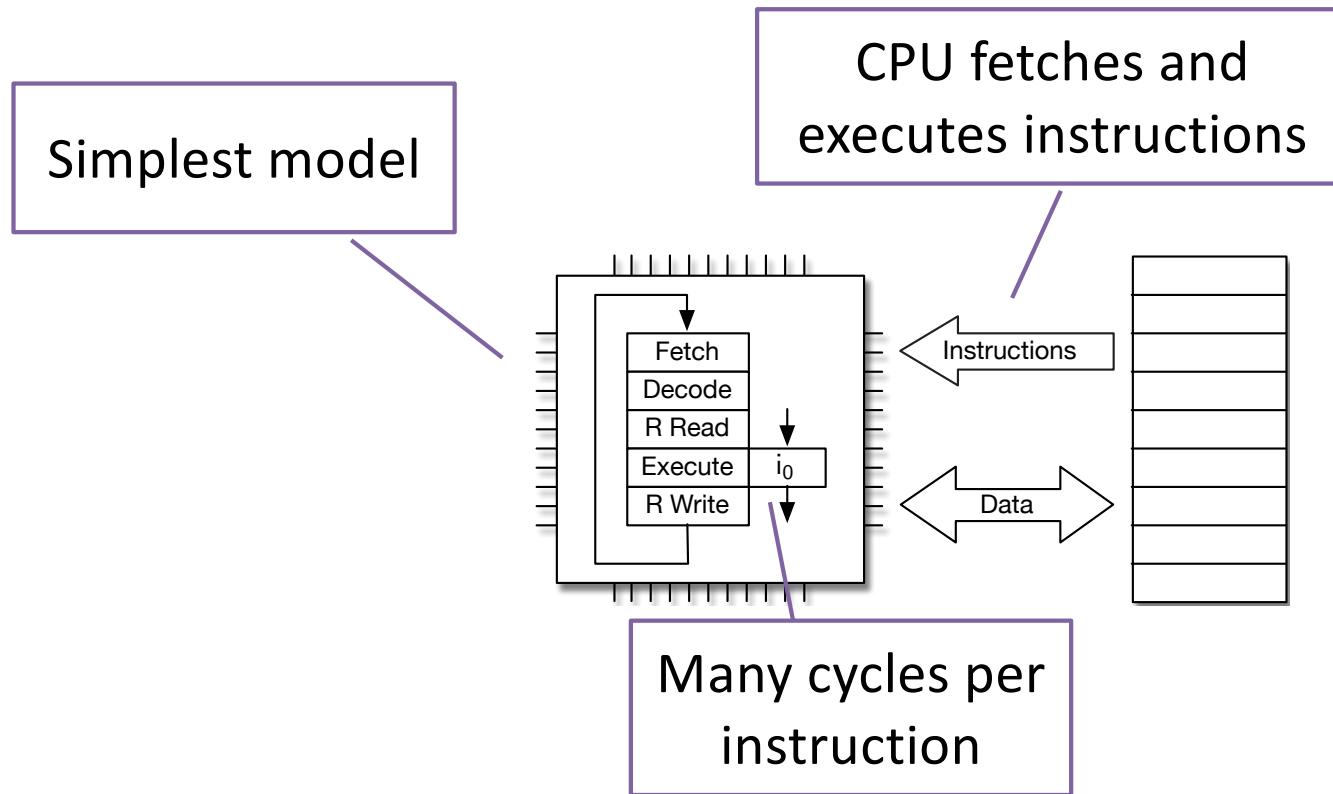
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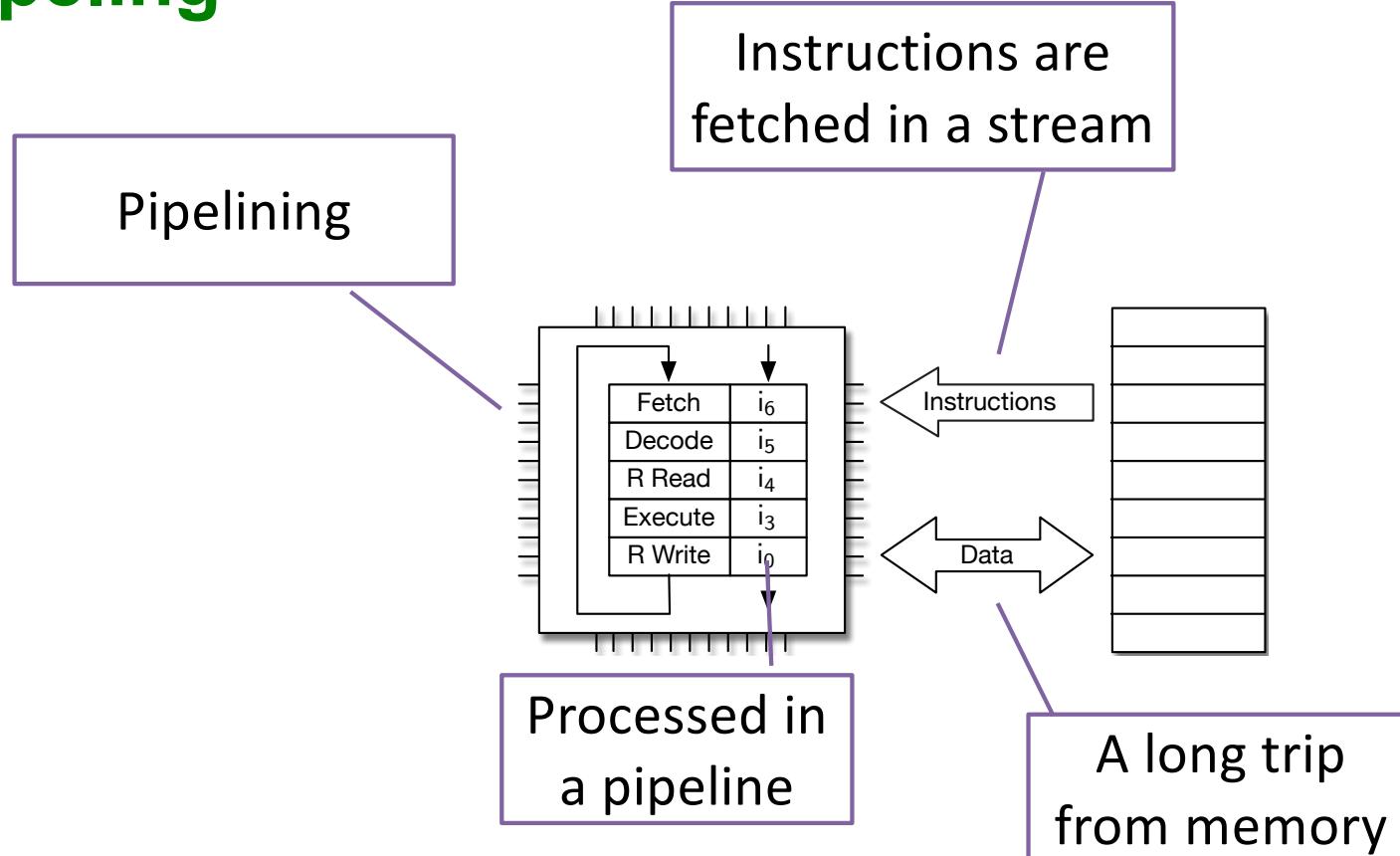
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Scaling progression of CPUs

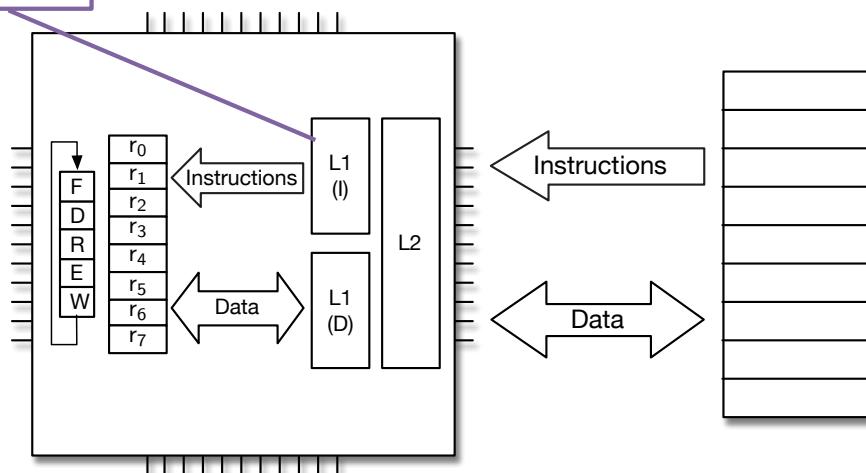


Pipelining



Hierarchical memory

Use special, fast
memory to keep data
and instructions close

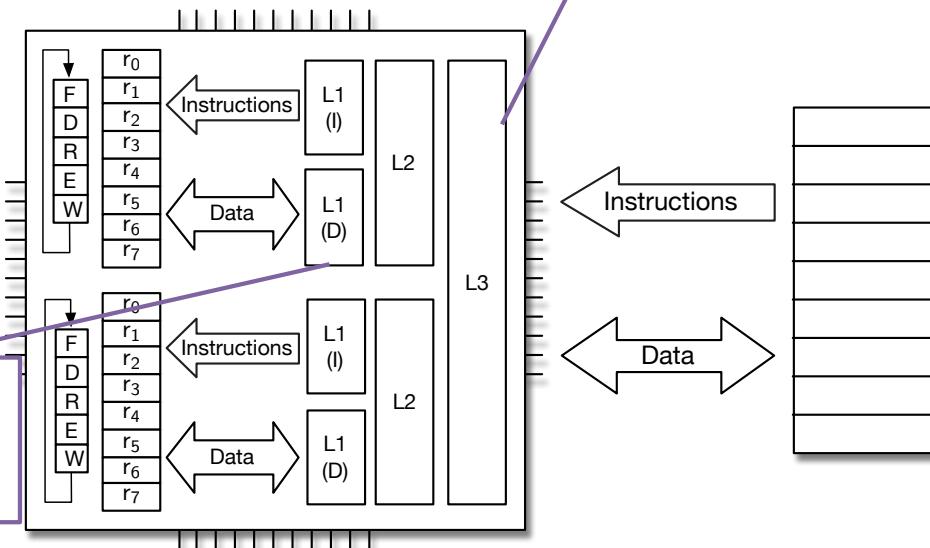


Multicore CPUs

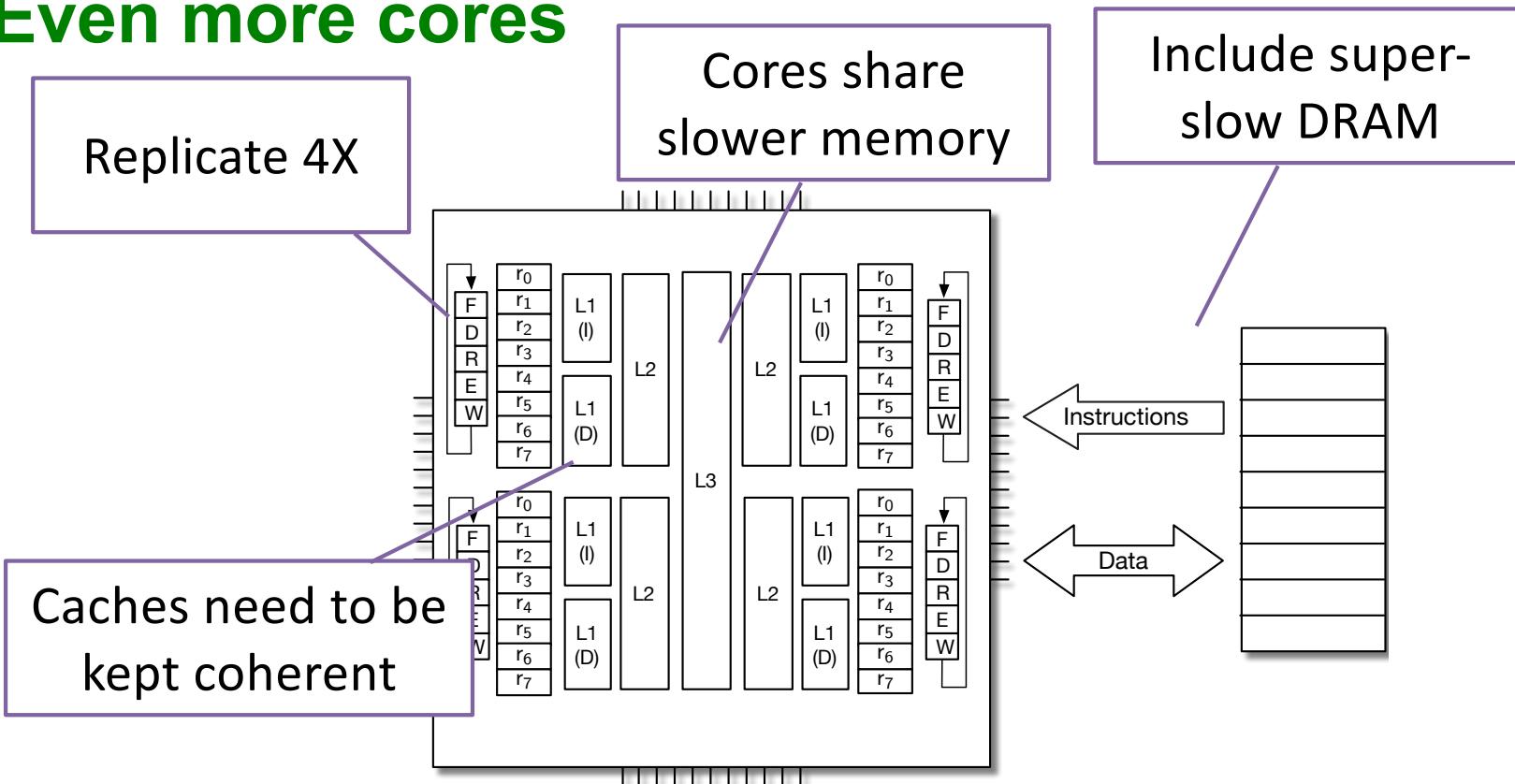
Replicate 2X

Cores share
slower memory

Caches need to be
kept coherent



Even more cores

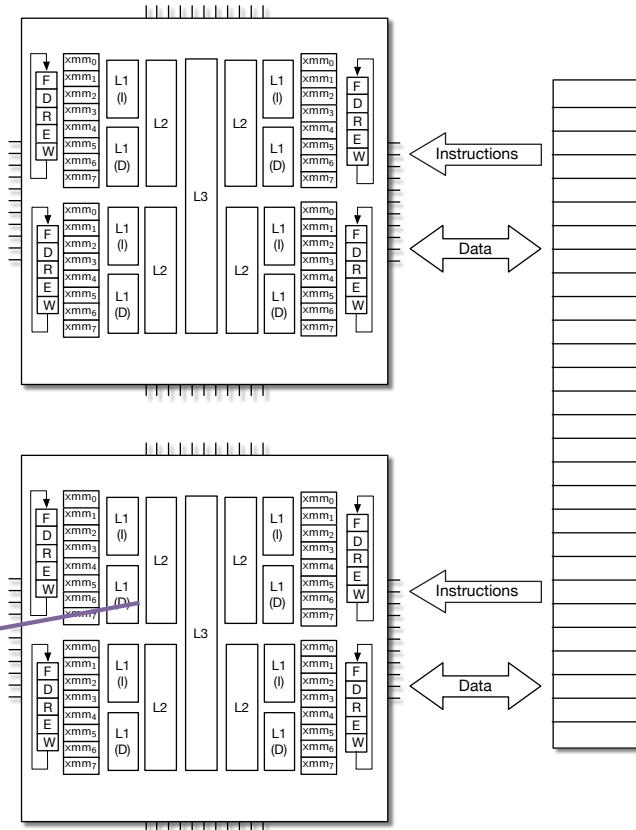


Symmetric Multi-Processor (SMP)

Multiple CPU chips

AKA “sockets”

Caches still need to be kept (somewhat) coherent



Memory may be uniformly shared among sockets

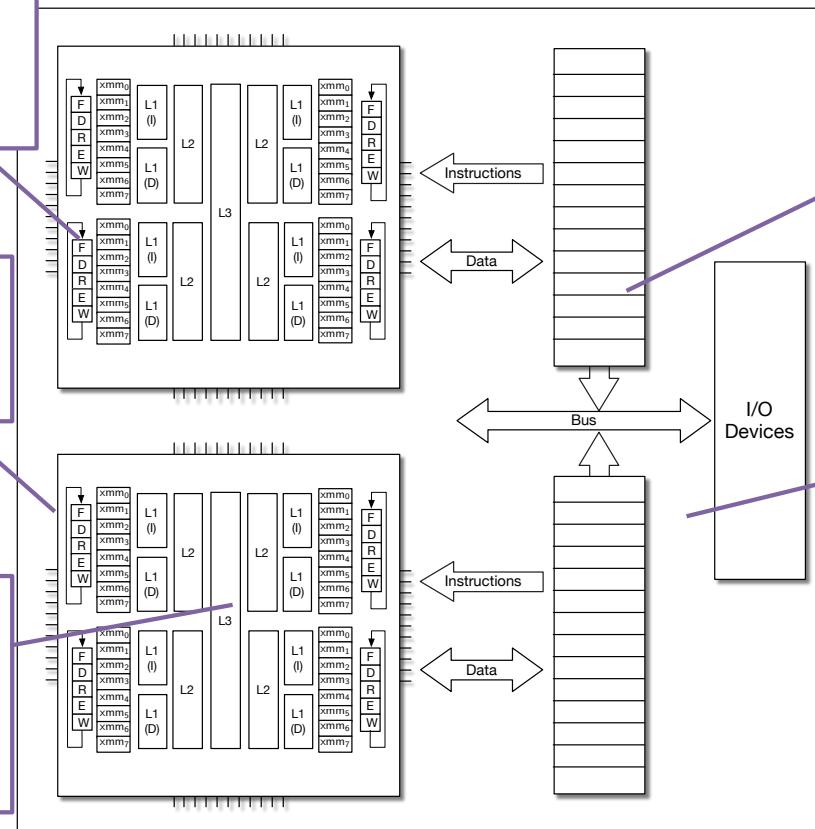
Uniform memory access (UMA)

Asymmetric

Multiple CPU chips

AKA “sockets”

Caches still need to be kept (somewhat) coherent: CC-NUMA



Memory may be non-uniformly shared among sockets

Non-uniform memory access (NUMA – most common)

Putting it All Together

Put sockets
on a blade

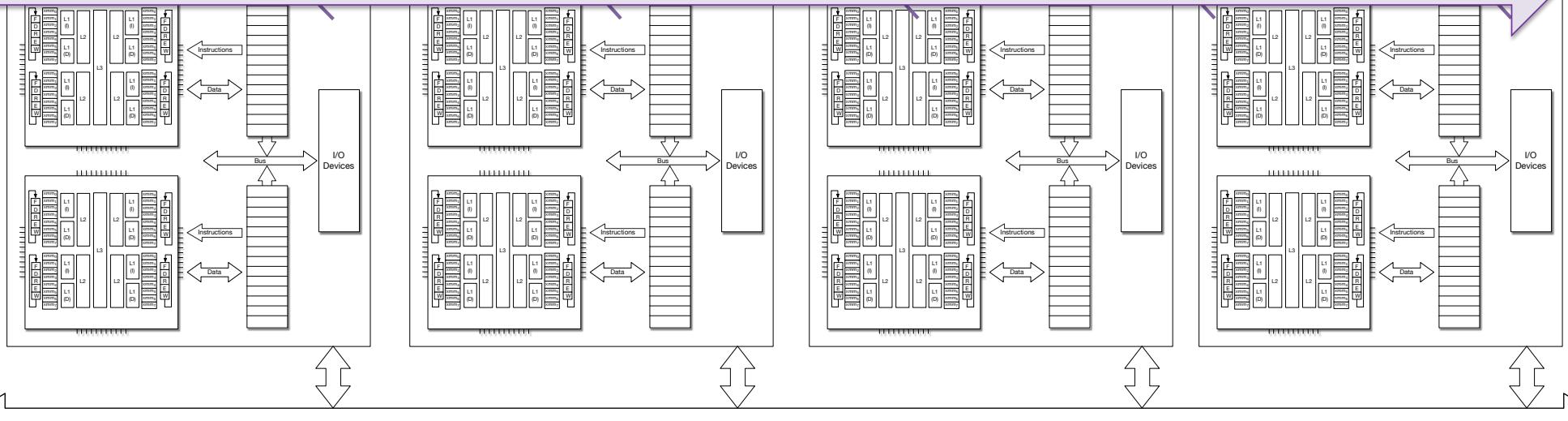
Put blades
in a chassis

Put chassis
in a rack

Put racks in
a center

Put centers
in the cloud

Our Path This Quarter



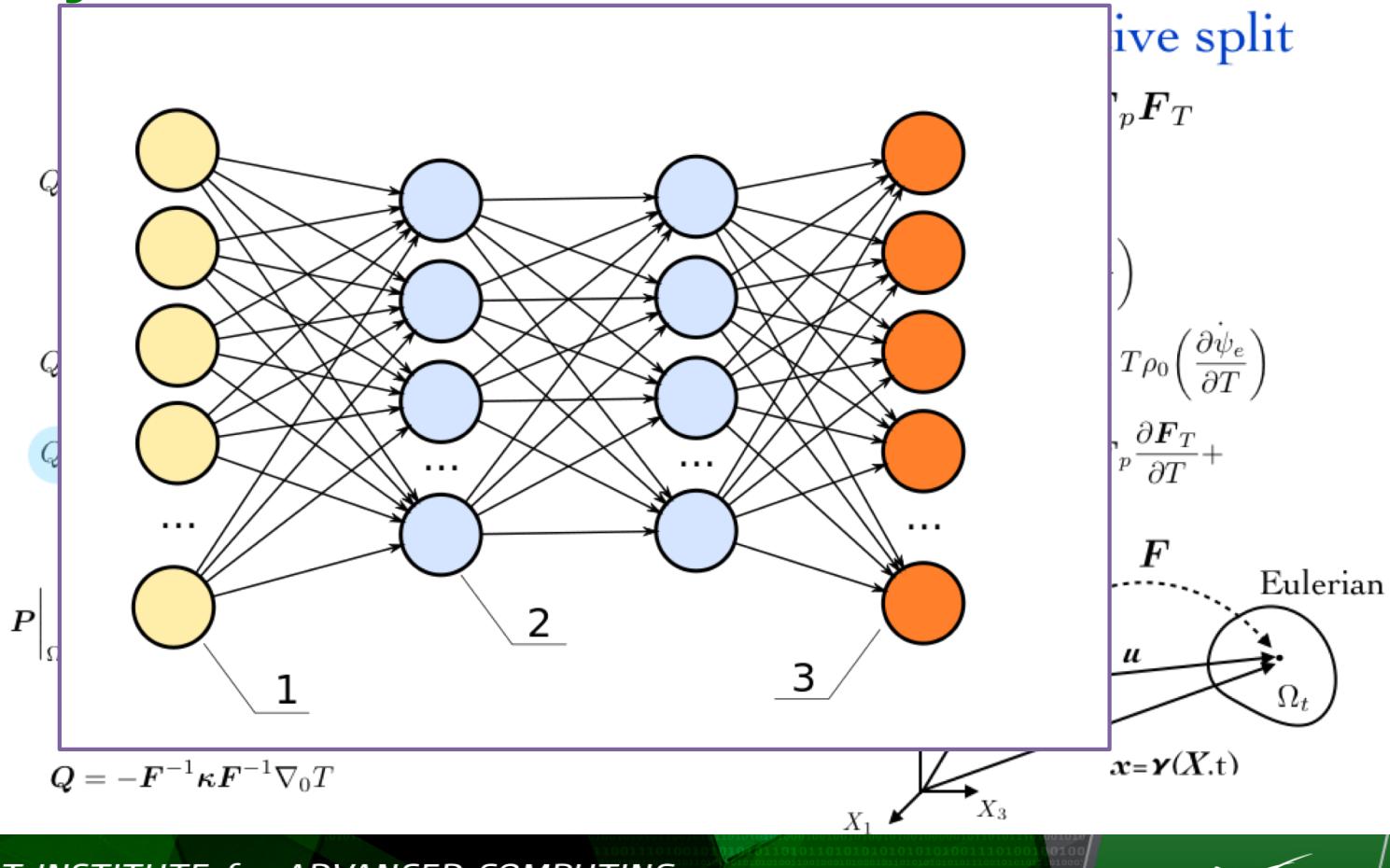
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Multiphysics Solver



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Putting it All Together

Put sockets
on a blade

Put blades
in a chassis

Put chassis
in a rack

Put racks in
a center

Put centers
in the cloud

Our Path This Quarter

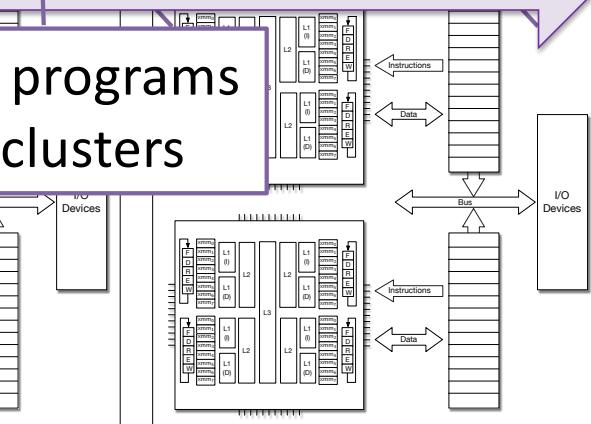
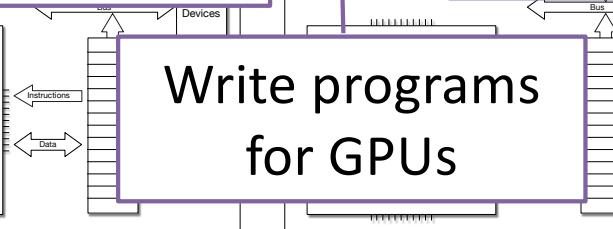
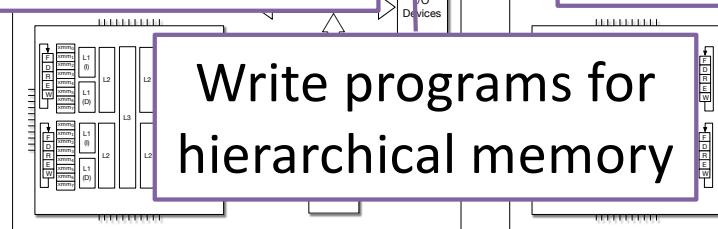
Write programs
for one core

Write programs
for multicore

Write programs
for clusters

Write programs for
hierarchical memory

Write programs
for GPUs



Write A Program

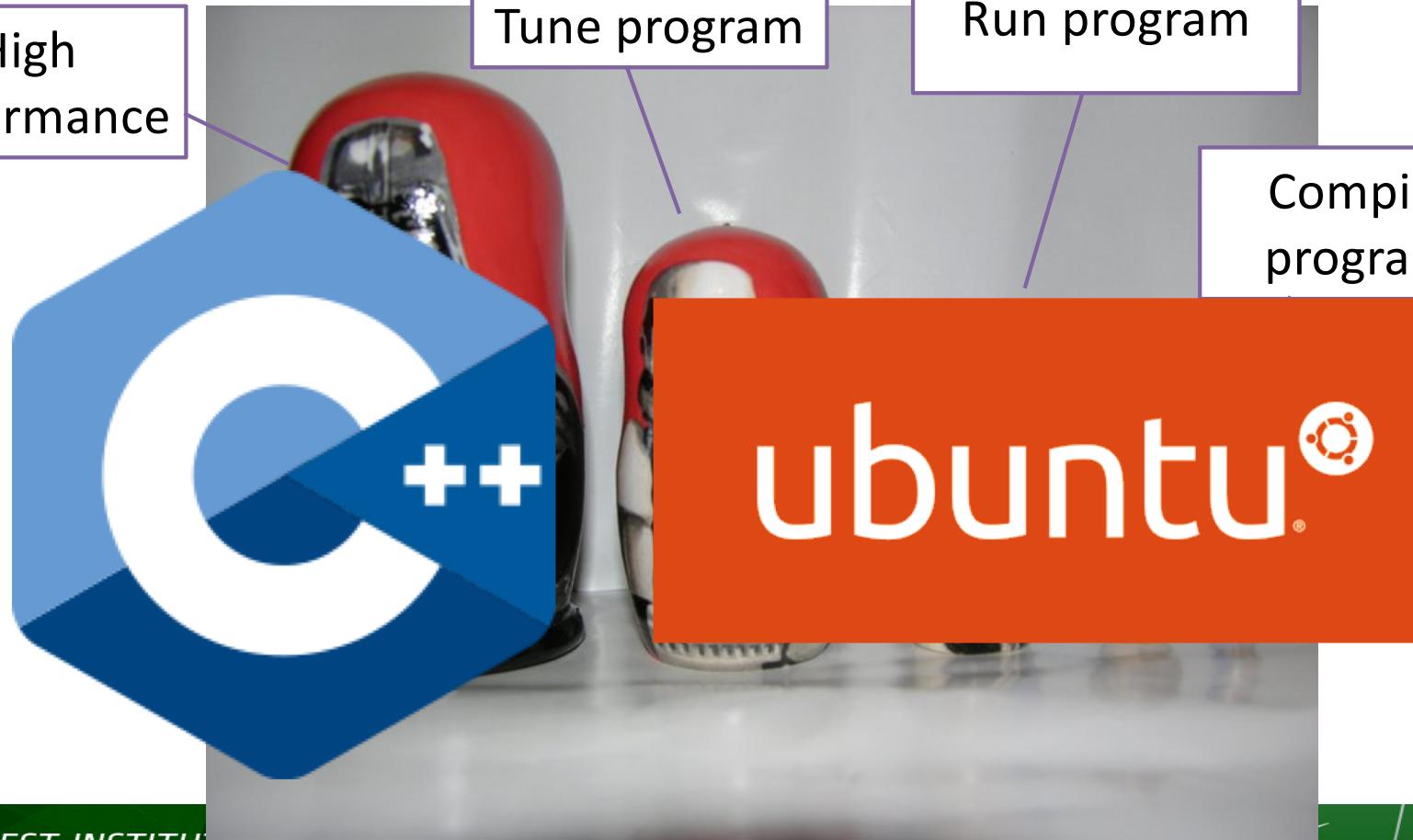
High performance

Measure and
Tune program

Run program

Compile
program

Write
program



Developing your code



- That includes (especially) mental labor
- Use productivity tools
- **VS code** (rec'd), Atom, Eclipse

A screenshot of the Visual Studio Code (VS Code) interface. On the left, the Extensions sidebar shows popular extensions like C#, Python, Debugger for Chrome, C/C++, Go, ESLint, and PowerShell. The main workspace shows a TypeScript file named 'app.ts' and 'www.ts'. The code in 'www.ts' is:

```
1 import app from './app';
2 import debugModule = require('debug');
3 import http = require('http');
4
5 const debug = debugModule('node-express-typescript:server');
6
7 // Get port from environment and store in Express.
8 const port = normalizePort(process.env.PORT || '3000');
9 app.set('port', port);
10
11 // create
12 const server = app.listen(port, () => {
13   console.log(`Server listening on port ${port}`);
14 });
15
16 server.on('error', (err) => {
17   if (err.syscall === 'listen') {
18     let bind = `Port ${port}`;
19     if (err.code === 'EADDRINUSE') {
20       console.error(`${bind} is already in use!`);
21     } else {
22       console.error(`Error: ${bind} ${err.message}`);
23     }
24   } else {
25     console.error(`Error: ${err.message}`);
26   }
27 });
28
29
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```

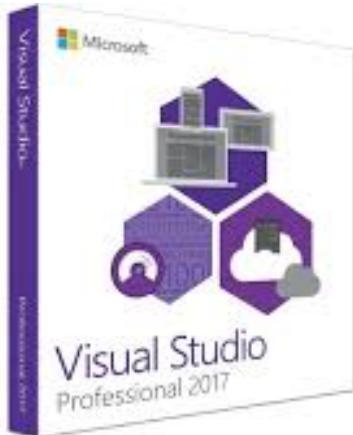
The status bar at the bottom indicates: master, 1131, 0, Ln 9, Col 21, Spaces: 2, UTF-8, LF, TypeScript, and a smiley face icon.

The AMATH 483/583 Development Environment

- Windows 10 (Pro and Education) and Mac OS X can be made to approximate Linux
 - Windows Subsystem for Linux (configured per course guidelines)
 - Xcode command-line tools (configured per course guidelines)
- How-to documentation in problem set and on line

A screenshot of the Microsoft Visual Studio Code (VS Code) interface. The main area shows a code editor with the file `www.ts` open, containing TypeScript code for a node.js application. The code includes imports for `app`, `debugModule`, and `http`, and defines a `normalizePort` function. The left sidebar shows the "EXTENSIONS" view with several popular extensions listed, including C#, Python, Debugger for Chrome, C/C++, Go, ESLint, and PowerShell. The bottom status bar indicates the file is in "master", has 11131 changes, 0 errors, and 0 warnings, and is using UTF-8 encoding.

What about ...?



- Muscle memory for typing is not the same as productivity (know the difference)
 - Stretch yourself
- Use any environment where you are most productive
- We can only support one (VS code + clang + “Linux”)
- Assignments must work with autograder

shells

- sh: “Bourne shell” (Stephen Bourne, Bell Labs c.1977)
- ksh: Korn shell (David Korn, Bell Labs, c. 1983)
- csh: C shell (Bill Joy, UC Berkeley, 70s)
 - and cousin tcsh – which is what I use
- bash (Brian Fox, 1989)
 - who knows what this stands for (without searching)
- All are Linux (Unix) processes with read-eval-print loops
- But also complete systems scripting language for dealing with Unix
 - Unix philosophy: data in text format, small programs using text I/O

Bourne again
shell

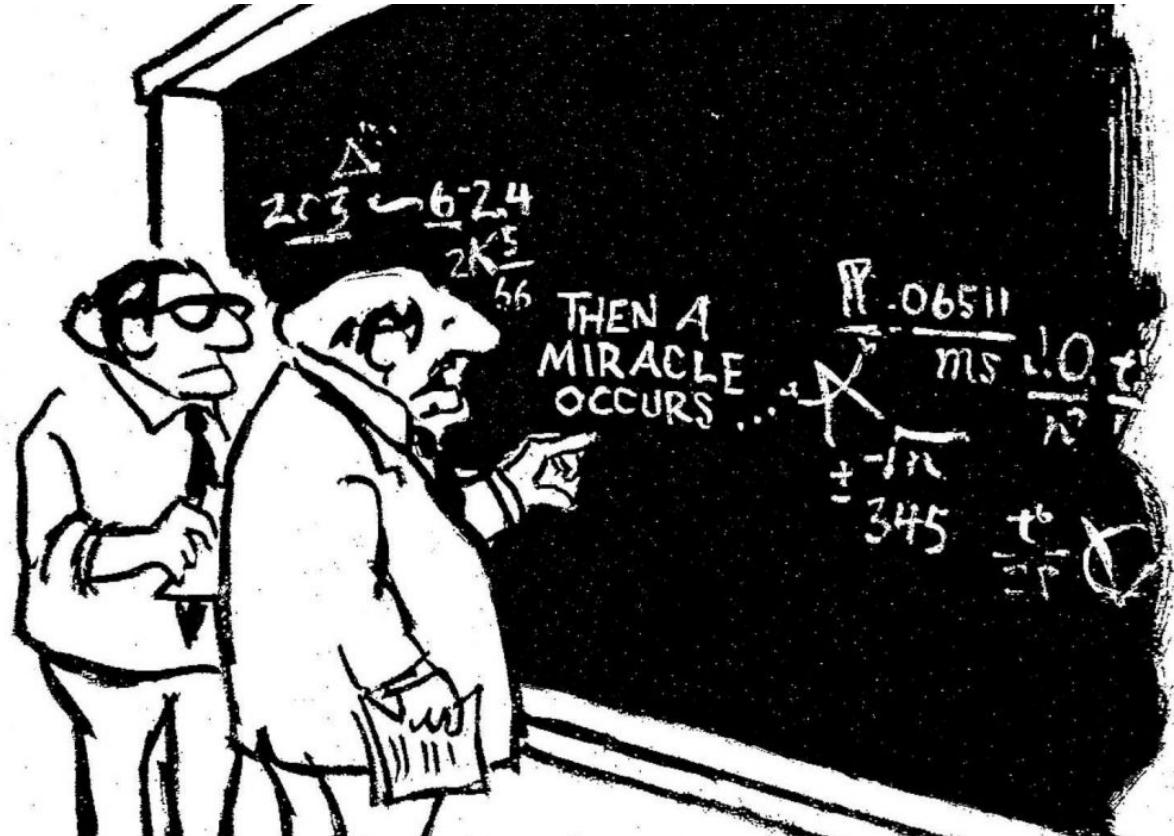
Programs and Programming

```
int main() {  
    int a = 1;  
    double x = 0.3;  
    foo(x, a);  
}
```

?



Programs and Programming



© S. Harris

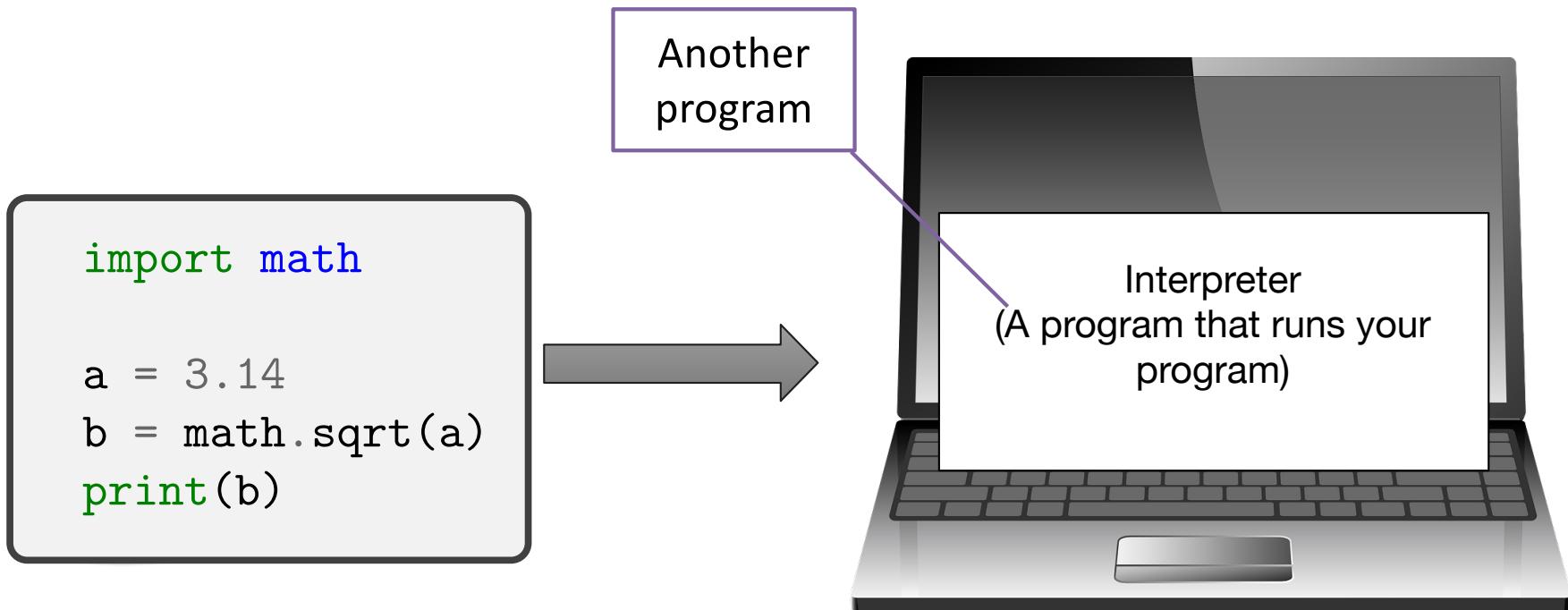
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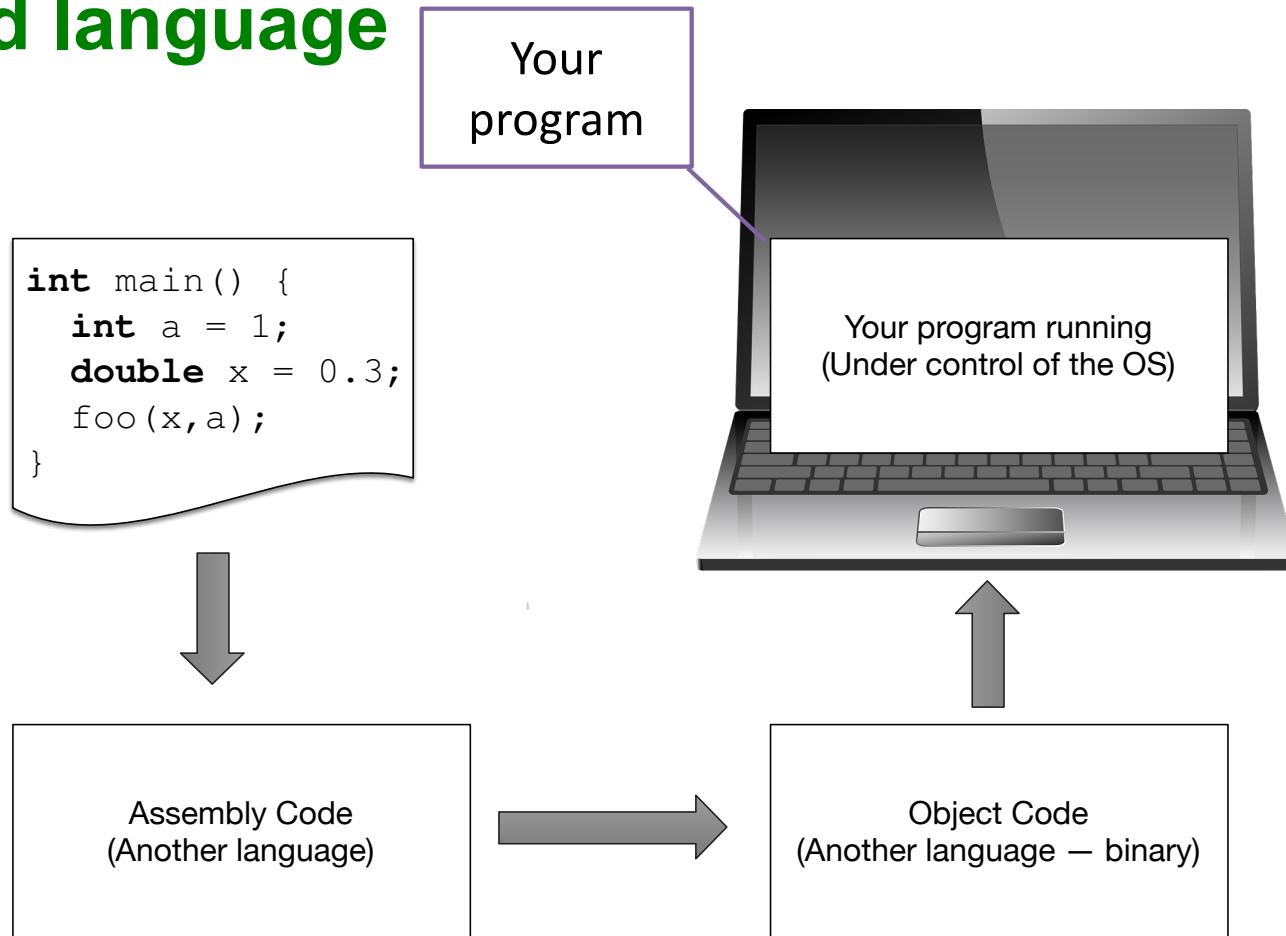
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Interpreted language (Python)



Compiled language



Interpreted vs compiled

Use math library

Call function from math library

Use functions from iostream library

Use math library

```
import math  
  
a = 3.14  
b = math.sqrt(a)  
print(b)
```

Curly braces for code blocks

Code must be in a function

Declare variables

Print result

Variables are typed

int main()

double a = 3.14;
double b = std::sqrt(a);

std::cout << b << std::endl;
return 0;

}

#include <cmath>
<iostream>

Call function

"std" rather than "math"

Compilation

```
#include <cmath>
#include <iostream>

int main() {
    double a = 3.14;
    double b = std::sqrt(a);
    std::cout << b << std::endl;

    return 0;
}
```

You can't run
this code

It needs to be
turned into code
that can run

An
“executable”

Multi-step
process

Compile to
object file

Bits just for
this code

Then link in
libraries for
sqrt and IO

Compiling

- To compile one source file to an executable
 - \$ c++ filename.cpp
 - (What is the name of the executable?)
- To compile multiple source files to an executable
 - \$ c++ one.cpp two.cpp three.cpp
- To create an object file
 - \$ c++ -c one.cpp –o one.o
- To create an executable from multiple object files
 - \$ c++ one.o two.o three.o –o myexecutable

Slice of C++

- C++11 (C++14, C++17, C++20) are quite modern languages
- But C++11 (et al) and libraries are *huge*
- We will use a focused slice of C++11
- Use some modern features
- Avoid legacy features (such as pointers)
- Avoid modern features (OO)

```
#include <cmath>
#include <iostream>

int main() {
    double a = 3.14;
    double b = std::sqrt(a);
    std::cout << b << std::endl;

    return 0;
}
```

C++ development philosophy

P.1: Express ideas directly in code

P.2: Write in ISO Standard C++

P.3: Express intent

P.4: Ideally, a program should be statically type safe

P.5: Prefer compile-time checking to run-time checking

P.6: What cannot be checked at compile time should be checkable at run time

P.7: Catch run-time errors early

P.8: Don't leak any resources

P.9: Don't waste time or space

P.10: Prefer immutable data to mutable data

P.11: Encapsulate messy constructs, rather than spreading through the code

P.12: Use supporting tools as appropriate

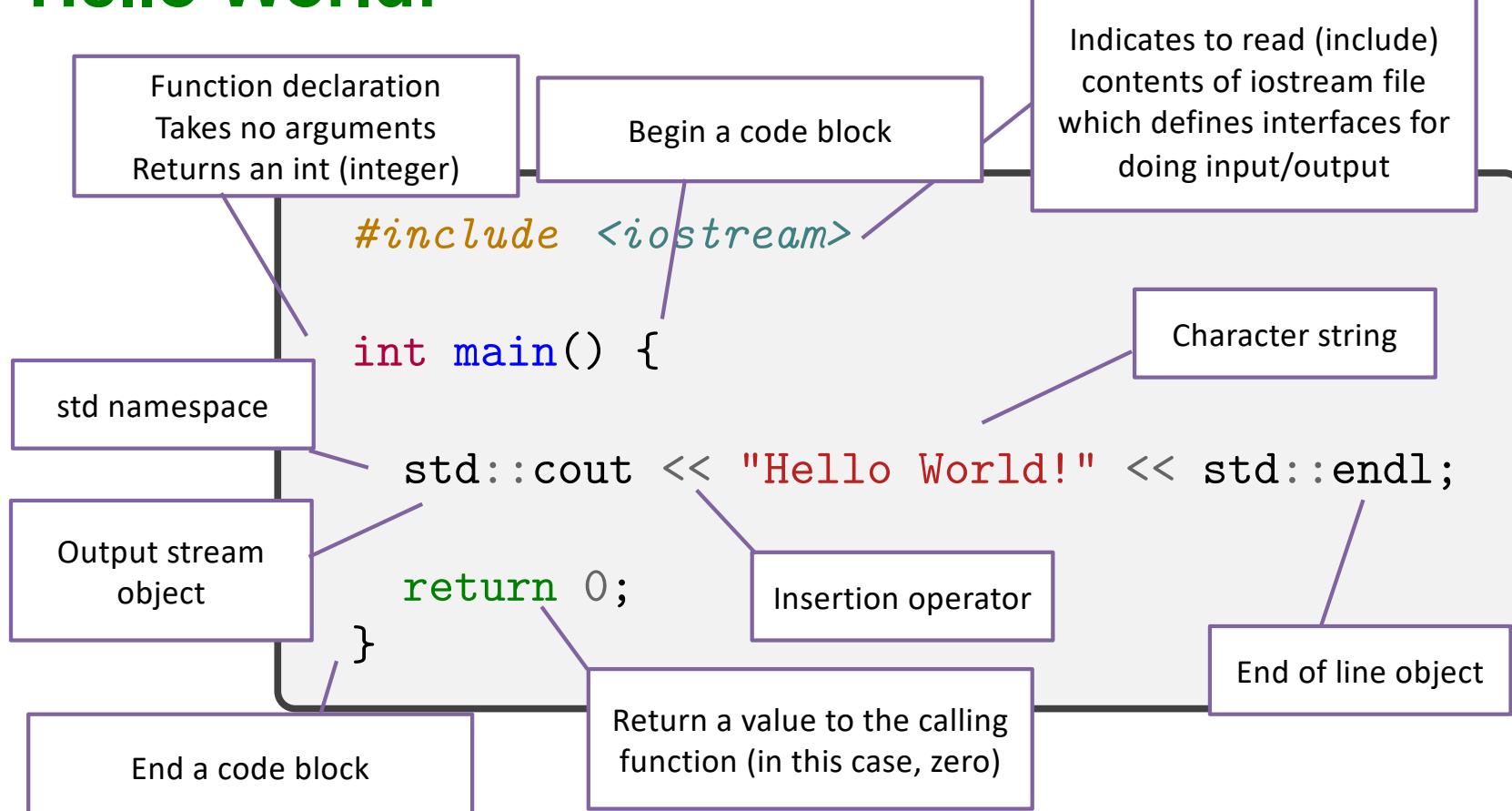
P.13: Use support libraries as appropriate

Only one rule
about C++

From C++ Core
Guidelines

Many follow
from the two
simple rules

Hello World!



#include

- Pulls text of <file> into source file
- Usually contain declarations and definitions of types, functions, etc
 - External libraries or other source files

```
//  
  
int main() {  
  
    std::cout << "Hello World!" <<  
  
    return 0;  
}
```

No includes

```
$ g++ hello.cpp  
hello.cpp:3:3: error: use of undeclared identifier 'std'  
    std::string message = "Hello World";  
           ^  
  
hello.cpp:4:3: error: use of undeclared identifier 'std'  
    std::cout << message << std::endl;  
           ^  
  
hello.cpp:4:27: error: use of undeclared identifier 'std'  
    std::cout << message << std::endl;  
                           ^  
  
3 errors generated.
```

Comments

```
// This is a comment
/*
    This is also a comment
*/
// This is a
// multiline comment
int main() {

    std::cout << "Hello World!" << std::endl

    return 0; // main should always return 0
}
```

Delimit to end of line using //

Can also use C-style /* */ (discouraged)

Style for multiline comments

In-line comments

#include

- Pulls text of <file> into source file
- Usually contain declarations and definitions of types, functions, etc
 - External libraries or other source files

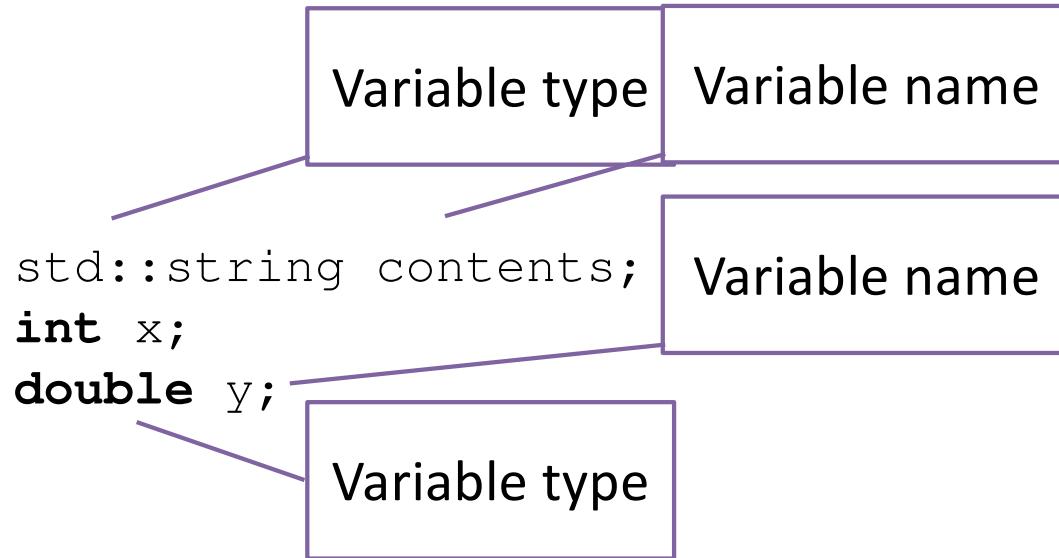
```
#include <algo>
Wrong include

int main() {
    std::cout << "Hello World!" << std::end
    return 0; // main should always return
}
```

```
$ c++ aa.cpp
aa.cpp:5:8: error: no type named 'string' in namespace 'std'
    std::string message = "Hello World";
           ^~~~~~
aa.cpp:6:8: error: no member named 'cout' in namespace 'std'; did you mean
    std::cout << message << std::endl;
           ^~~~~~^~~~
count
/usr/bin/../lib/gcc/x86_64-linux-gnu/5.4.0/../../../../include/c++/5.4.0/bits
    'count' declared here
    count(_InputIterator __first, _InputIterator __last, const _Tp& __value)
      ^
aa.cpp:6:32: error: no member named 'endl' in namespace 'std'
    std::cout << message << std::endl;
           ^~~~~~^
3 errors generated.
```

Types

- Variable definition



- C++ has many **built-in** types: int, double, char, etc
- Other types are defined for **libraries** (accessed via #include)
- Almost always **class** definitions

Declaring and Initializing Variables

- In the old days variables were declared at the beginning of a block

```
int main() {  
    double x, y; ————— Declaration  
    // ...  
    x = 3.14159;  
    y = x * 2.0; ————— Use  
    // ...  
    return 0;  
}
```

- Now they can be defined anywhere in the block

```
int main() {  
    // ...  
    double x = 3.14159;  
    double y = x * 2.0;  
    // ...  
    return 0; ————— Declaration with initialization  
}
```

- Best practice: Don't declare variables before they are needed and **always** initialize if possible

Namespaces

```
#include <iostream>

double pi = 3.14;

int main() {

    std::cout << "The legislated value of pi is ";
    std::cout << pi << std::endl;

    return 0;
}
```

\$./a.out

The legislated value of pi is 3.14

To print this value

Compiler needs to
resolve this symbol

Namespaces

```
#include <iostream>

namespace amath583 {
    double pi = 3.14;
}

int main() {
    std::cout << "The legislated value of pi is "
    std::cout << pi << std::endl;

    return 0;
}
```

```
ns.cpp:11:16: error: use of undeclared identifier 'pi'; did you mean 'amath583::pi'?
    std::cout << pi << std::endl;
               ^~~
               amath583::pi
ns.cpp:5:10: note: 'amath583::pi' declared here
    double pi = 3.14;
               ^
1 error generated.
```

pi is hidden in a namespace

But can't

Compiler needs to resolve this symbol

Namespaces

```
#include <iostream>

namespace amath583 {
    double pi = 3.14;
}

int main() {
    std::cout << "The legislated value of pi is ";
    std::cout << amath583::pi << std::endl;

    return 0;
}
```

```
$ ./a.out
The legislated value of pi is 3.14
```

Look for the variable
pi in the amath583
namespace

Namespaces

```
#include <iostream>

namespace amath583 {
    double pi = 3.14;
}

using amath583::pi;

int main() {

    std::cout << "The legislated value of pi is ";
    std::cout << pi << std::endl;

    return 0;
}
```

We can also tell the compiler to look for pi in the namespace this way

```
$ ./a.out
The legislated value of pi is 3.14
```

Use “pi” where it can be found
(no specified namespace)

Namespaces

```
#include <iostream>

namespace amath583 {
    double pi = 3.14;
}
```

Everything in this namespace can be found

```
using amath583;

int main() {
```

Open the namespace

```
    std::cout << "The legislated value of pi is ";
    std::cout << pi << std::endl;

    return 0;
}
```

Use “pi” where it can be found

Namespaces

```
#include <iostream>

namespace amath483 {
    double pi = 3.14159;
}

namespace amath583 {
    double pi = 3.14;
}

int main() {

    std::cout << "The legislated value of pi is ";
    std::cout << pi << std::endl;

    return 0;
}
```

```
n2.cpp:18:16: error: reference to 'pi' is ambiguous
    std::cout << pi << std::endl;
               ^
n2.cpp:5:10: note: candidate found by name lookup is 'amath483::pi'
    double pi = 3.14159;
               ^
n2.cpp:9:10: note: candidate found by name lookup is 'amath583::pi'
    double pi = 3.14;
               ^
1 error generated.
```

What happens here?

Can't find pi

How to resolve
ambiguity?

Namespaces

```
#include <iostream>

namespace amath483 {
    double pi = 3.14159;
}

namespace amath583 {
    double pi = 3.14;
}

using namespace amath483::pi;

int main() {

    std::cout << "The legislated value of pi is ";
    std::cout << pi << std::endl;

    return 0;
}
```

\$./a.out

The legislated value of pi is 3.14159

Specify that this pi is in
the global namespace

Namespaces

```
#include <iostream>

namespace amath483 {
    double pi = 3.14159;
}

namespace amath583 {
    double pi = 3.14;
}

using namespace amath483::pi;

int main() {

    std::cout << "The legislated value of pi is ";
    std::cout << amath583::pi << std::endl;

    return 0;
}
```

```
$ ./a.out
The legislated value of pi is 3.14
```

(This one)

Specify exactly which pi

Namespaces

```
#include <iostream>

namespace amath483 {
    double pi = 3.14159;
}

namespace amath583 {
    double pi = 3.14;
}

using namespace amath483::pi;

int main() {

    std::cout << "The legislated value of pi is ";
    std::cout << amath583::pi << std::endl;

    return 0;
}
```

(This one)

Specify exactly which pi

Disambiguating

```
#include <iostream>
```

```
namespace amath483 {  
    double pi = 3.14159;  
};
```

```
namespace amath583 {  
    double pi = 3.14;  
};
```

```
double pi = 3.141592653589793238462643383279502884197;
```

```
int main() {  
  
    std::cout << "The value of pi is ";  
    std::cout << pi << std::endl;  
  
    return 0;  
}
```

```
$ ./a.out  
The value of pi is 3.14159
```

This one. (Why?)

Which pi?

Disambiguating

```
#include <iostream>

namespace amath483 {
    double pi = 3.14159;
}

namespace amath583 {
    double pi = 3.14;
}

double pi = 3.141592653589793238462643383279502884197;

using namespace amath483;
using namespace amath583;

int main() {

    std::cout << "The value of pi is ";
    std::cout << pi << std::endl;

    return 0;
}
```

```
$ ./a.out

pi4.cpp:19:16: error: reference to 'pi' is ambiguous
    std::cout << pi << std::endl;
               ^
pi4.cpp:11:8: note: candidate found by name lookup is 'pi'
double pi = 3.141592653589793238462643383279502884197;
               ^
pi4.cpp:8:10: note: candidate found by name lookup is 'amath583::pi'
    double pi = 3.14;
               ^
pi4.cpp:4:10: note: candidate found by name lookup is 'amath483::pi'
    double pi = 3.14159;
               ^
1 error generated.
```

We know how to disambiguate
and pick these

What about the global pi?

Which pi?

The global namespace

```
#include <iostream>
```

```
namespace amath483 {  
    double pi = 3.14159;  
};
```

```
namespace amath583 {  
    double pi = 3.14;  
};
```

```
double pi = 3.1415926535
```

```
using namespace amath483  
using namespace amath583
```

```
int main() {  
  
    std::cout << "The value of pi is "  
    std::cout << ::pi << std::endl;  
  
    return 0;  
}
```

```
$ ./a.out  
The value of pi is 3.14159
```

Explicitly state which pi

Global namespace

The global namespace

```
#include <iostream>
#include <iomanip>

namespace amath483 {
    double pi = 3.14159;
}

namespace amath583 {
    double pi = 3.14;
}

double pi = 3.141592653589793238462643383279502884197;

using namespace amath483;
using namespace amath583;

int main() {
    std::cout << "The value of pi is ";
    std::cout << std::setprecision(15) << ::pi << std::endl;

    return 0;
}
```

\$./a.out
The value of pi is 3.14159265358979

Include iomanip

Set precision to 15 digits

So what about namespace std?

```
#include <iostream>

namespace amath483 {
    double pi = 3.14159;
}

namespace amath583 {
    double pi = 3.14;
}

void foo() {
    using namespace amath583;
    std::cout << "The legislated value of pi is ";
    std::cout << pi << std::endl;
}

void bar() {
    using namespace amath483;
    std::cout << "The legislated value of pi is ";
    std::cout << pi << std::endl;
}

int main() {
    foo(); bar();
    return 0;
}
```

Local scope

Local scope

- C++ core guidelines:
Use using
namespace directives for
transition, for foundation
libraries (such as std), or
within a local scope
- Resist using namespace
directives globally
- Don't write using
namespace in a header file

First option for AMATH 483/583

```
#include <iostream>
#include <string>

int main() {

    std::string message = "Hello World";
    std::cout << message << std::endl;

    return 0;
}
```

Explicitly use variables
from namespace std

Second option for AMATH 483/583

```
#include <iostream>
using std::cout;  using std::endl;
using std::string;

int main() {

    string message = "Hello World";
    cout << message << endl;

    return 0;
}
```

Using for just the variables you want

Third options for AMATH 483/583

```
#include <iostream>
using namespace std;

int main() {

    string message = "Hello World";
    cout << message << endl;

    return 0;
}
```

Open all of
namespace std

Which option for AMATH 483/583

P.3: Express intent

```
#include <iostream>
#include <string>

int main() {
    std::string message = "Hello World";
    std::cout << message << std::endl;

    return 0;
}
```

Organizing your programs

- Software development is difficult
- How do humans attack complex problems?
- Apply the same principles to software
- Modular / reusable
- Well defined interfaces and functionality
- Understandable



Newton's Method for Square Root

- To solve $f(x) = 0$ for x
- Linearize (approximate the nonlinear problem with a linear one) and solve the linear problem
- Iterate
- Taylor: $f(x + \Delta x) \approx f(x) + \Delta x f'(x) = \Delta x f'(x)$

$$\Delta x = -\frac{f(x)}{f'(x)}$$

$$f(x) = x^2 - y = 0 \rightarrow y = \sqrt{x} \quad f'(x) = 2x \quad \Delta x = -\frac{x^2 - y}{2x}$$

NORTHWEST INSTITUTE for ADVANCED COMPUTING

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University of Washington by Andrew Lumsdaine

Pacific Northwest
NATIONAL LABORATORY
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Compute square root of 2

```
#include <iostream>
#include <cmath>

int main () {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-2.0) / (2.0*x) ;
        x += dx;
        if (std::abs(dx) < 1.e-9) break;
    }

    std::cout << x << std::endl;

    return 0;
}
```

Compute square root of 3

```
#include <iostream>
#include <cmath>

int main () {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-3.0) / (2.0*x) ;
        x += dx;
        if (std::abs(dx) < 1.e-9) break;
    }

    std::cout << x << std::endl;

    return 0;
}
```

Compute square root of 2 and 3

```
#include <iostream>
#include <cmath>

int main () {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-2.0) / (2.0*x) ;
        x += dx;
        if (std::abs(dx) < 1.e-9) break;
    }

    std::cout << x << std::endl;

    return 0;
}
```

Don't do the same thing twice in different places

```
#include <iostream>
#include <cmath>

int main () {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-3.0) / (2.0*x) ;
        x += dx;
        if (std::abs(dx) < 1.e-9) break;
    }

    std::cout << x << std::endl;

    return 0;
}
```

But they're not exactly the same

This is the only difference

This is the only difference

Procedural Abstraction

```
#include <cmath>
double sqrt583(double y) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-y) / (2.0*x);
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }
    return x;
}
```

It returns a double

It returns a double

Define function named sqrt583

The function is **parameterized** by y

Which is a double

Same code as before

Except for parameterization

Procedural Abstraction

It returns
a double

It returns
a double

```
#include <cmath>

double sqrt583(double y) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-y) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }
    return x;
}
```

Redundant?

Compiler can deduce return types

It returns
a double

It returns
a double

```
#include <cmath>

auto sqrt583(double y) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-y) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }
    return x;
}
```

Note auto is a
C++14 feature!

Square root of 2 and 3

Note initialization
and declaration of i

What is a size_t?

Pass
parameter 2

Pass
parameter 3

```
#include <iostream>
#include <cmath>

double sqrt583(double y) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-y) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }
}
```

```
int main () {
    sqrt583(2.0) << std::endl;
    sqrt583(3.0) << std::endl;
}
```

Thought experiment

Change value of y

Print y

What will print?

```
#include <iostream>
#include <cmath>

double sqrt583(double y) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-y) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }
    y = x;
    return x;
}

int main () {
    double y = 2.0;
    std::cout << sqrt583(y) << std::endl;
    std::cout << y << std::endl;

    return 0;
}
```

```
$ ./a.out
1.41421
2
```

Parameter Passing in C++

y is passed **by value** (copied), so only the copy is changed, not the original

C++ has “pass by value” semantics

```
#include <iostream>
#include <cmath>

double sqrt583(double y) {
    double x = 1.0;
    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-y) / (2.0*x);
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }
    y = x;
    return x;
}

int main () {
    double y = 2.0;
    std::cout << sqrt583(y) << std::endl;
    std::cout << y << std::endl;
    return 0;
}
```

Parameter Passing in C++

y is passed **by value** (copied), so only the copy is changed, not the original

C++ has “pass by value” semantics

Just to be clear, the parameter can have any name (don’t confuse with y declared in main)

```
#include <iostream>
#include <cmath>

double sqrt583(double z) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-z) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }
    z = x;
    return x;
}

int main () {
    double y = 2.0;
    std::cout << sqrt583(y) << std::endl;
    std::cout << y << std::endl;

    return 0;
}
```

Before

```
$ ./a.out  
1.41421  
2
```

```
#include <iostream>  
#include <cmath>  
  
double sqrt583(double z) {  
    double x = 1.0;  
  
    for (size_t i = 0; i < 32; ++i) {  
        double dx = - (x*x-z) / (2.0*x) ;  
        x += dx;  
        if (abs(dx) < 1.e-9) break;  
    }  
  
    z = x;  
  
    return x;  
}  
  
  
int main () {  
    double y = 2.0;  
    std::cout << sqrt583(y) << std::endl;  
    std::cout << y << std::endl;  
  
    return 0;  
}
```

After

```
$ ./a.out  
1.41421  
1.41421
```

```
#include <iostream>  
#include <cmath>  
  
double sqrt583(double& z) {  
    double x = 1.0;  
  
    for (size_t i = 0; i < 32; ++i) {  
        double dx = - (x*x-z) / (2.0*x) ;  
        x += dx;  
        if (abs(dx) < 1.e-9) break;  
    }  
  
    z = x;  
  
    return x;  
}  
  
  
int main () {  
    double y = 2.0;  
    std::cout << sqrt583(y) << std::endl;  
    std::cout << y << std::endl;  
  
    return 0;  
}
```

After

```
$ ./a.out  
1.41421  
1.41421
```

y is passed by reference (not copied), so the original is changed

This variable

Is this variable

```
#include <iostream>  
#include <cmath>  
  
double sqrt583(double& z) {  
    double x = 1.0;  
  
    for (size_t i = 0; i < 32; ++i) {  
        double dx = - (x*x-z) / (2.0*x) ;  
        x += dx;  
        if (abs(dx) < 1.e-9) break;  
    }  
  
    z = x;  
  
    return x;  
}  
  
  
int main () {  
    double y = 2.0;  
    std::cout << sqrt583(y) << std::endl;  
    std::cout << y << std::endl;  
  
    return 0;  
}
```

Thought experiment

This variable

Is this variable

Which isn't a variable

```
#include <iostream>
#include <cmath>

double sqrt583(double &z) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-z) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }

    z = x;

    return x;
}

int main () {
    std::cout << sqrt583(2.0) << std::endl;
    return 0;
}
```

```
sqrtr2.cpp:21:16: error: no matching function for call to 'sqrt583'
    std::cout << sqrt583(2.0) << std::endl;
               ^~~~~~

sqrtr2.cpp:4:8: note: candidate function not viable: expects an l-value for 1st argument
double sqrt583(double &z) {
^
1 error generated.
```

Thought experiment

Why would we want to pass a reference?

“Out parameters”

Efficiency (no copy)

How can we do this?

```
#include <iostream>
#include <cmath>

double sqrt583(double &z) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-z) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }
    z = x;

    return x;
}

int main () {
    std::cout << sqrt583(2.0) << std::endl;

    return 0;
}
```

Before

```
#include <iostream>
#include <cmath>

double sqrt583(double &z) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-z) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }

    z = x;

    return x;
}

int main () {

    std::cout << sqrt583(2.0) << std::endl;

    return 0;
}
```

After

```
#include <iostream>
#include <cmath>

double sqrt583(const double &z) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-z) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }

    z = x;

    return x;
}

int main () {

    std::cout << sqrt583(2.0) << std::endl;

    return 0;
}
```

After

Promise not to change z

A reference to a
constant is okay

```
#include <iostream>
#include <cmath>

double sqrt583(const double &z) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-z) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }

    z = x;

    return x;
}

int main () {
    std::cout << sqrt583(2.0) << std::endl;

    return 0;
}
```

Functions

- F.2: A function should perform a single logical operation
- F.3: Keep functions short and simple
- F.16: For “in” parameters, pass cheaply-copied types by value and others by reference to const
- F.17: For “in-out” parameters, pass by reference to non-const
- F.20: For “out” output values, prefer return values to output parameters

Thought experiment

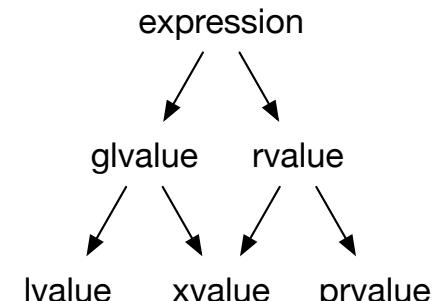
What's an l-value?

```
sqrtr2.cpp:21:16: error: no matching function for call to 'sqrt583'  
    std::cout << sqrt583(2.0) << std::endl;  
           ^~~~~~  
  
sqrtr2.cpp:4:8: note: candidate function not viable: expects an l-value for 1st argument  
double sqrt583(double &z) {  
    ^  
1 error generated.
```

```
#include <iostream>  
#include <cmath>  
  
double sqrt583(double &z) {  
    double x = 1.0;  
  
    for (size_t i = 0; i < 32; ++i) {  
        double dx = - (x*x-z) / (2.0*x) ;  
        x += dx;  
        if (abs(dx) < 1.e-9) break;  
    }  
  
    z = x;  
  
    return x;  
}  
  
int main () {  
    std::cout << sqrt583(2.0) << std::endl;  
    return 0;
```

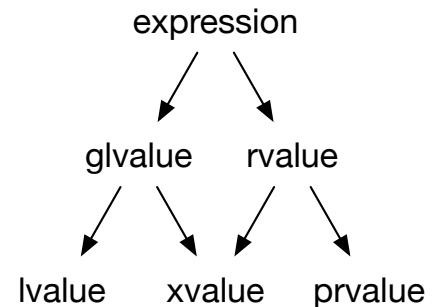
I-values and r-values

- Section 3.10 of C++ standard
 - A *glvalue* is an expression whose evaluation determines the identity of an object, bit-field, or function.
 - A *prvalue* is an expression whose evaluation initializes an object or a bit-field, or computes the value of the operand of an operator, as specified by the context in which it appears.
 - An *xvalue* is a glvalue that denotes an object or bit-field whose resources can be reused (usually because it is near the end of its lifetime).
 - An *lvalue* is a glvalue that is not an xvalue.
 - An *rvalue* is a prvalue or an xvalue



I-values and r-values

- More intuitively
- Ignore glvalue, xvalue, prvalue
- Ivalue is something that can go on the **left** of an assignment (correctly)
 - “Lives” beyond an expression
- Rvalue is something that can go on the **right** of an assignment (correctly)
 - Does not “live” beyond an expression



I-values and r-values

```
double x, y, z;
```

```
x = y;  
x = 1.0;  
y = x + z;
```

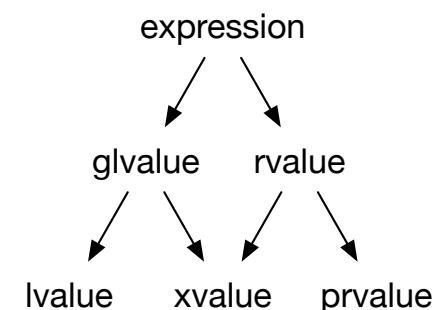
lvalue

rvalue

```
double x, y, z;
```

```
x = y;  
1.0 = x;  
x + z = y;
```

```
% c++ sl7.cpp  
c++ sl7.cpp  
sl7.cpp:7:9: error: expression is not assignable  
    x + z = y;  
    ~~~~~ ^  
1 error generated.
```



I-values and r-values

- Consider following program:

```
int main() {  
    double y = 2.0, z = 3.0;  
  
    double x = sqrt583(y+z);  
  
    return 0;  
}
```

rvalue

Copy: $x = y + z$ (lvalue = rvalue)

- With following declarations:

```
double sqrt583(double x);
```

OK to copy rvalue

```
double sqrt583(double& x);
```

Not OK to reference rvalue

```
double sqrt583(const double& x);
```

OK to reference const rvalue

I-values and r-values

- How is the value used in the function

```
double sqrt583(double y) {  
    double x = 0.0, dx;  
  
    do {  
        dx = - (x*x-y) / (2.0*x);  
        x += dx;  
    } while (abs(dx) > 1.e-9);  
  
    y = x; // lvalue  
  
    return x;  
}
```

- With following declarations:

```
double sqrt583(double x);
```

OK to copy rvalue

```
double sqrt583(double& x);
```

Not OK to reference rvalue

```
double sqrt583(const double& x);
```

OK to reference const rvalue

I-values and r-values

- How is the value used in the function

```
double sqrt583(double& y) {  
    double x = 0.0, dx;  
  
    do {  
        dx = - (x*x-y) / (2.0*x);  
        x += dx;  
    } while (abs(dx) > 1.e-9);  
  
    y = x;  
    return x;  
}
```

Ivalue ref

Ivalue ref

- With following declarations:

```
double sqrt583(double x);
```

Temp result of x+y is references

```
double sqrt583(double& x);
```

Not OK to reference rvalue

```
double sqrt583(const double& x);
```

I-values and r-values

- How is the value used in the function

```
double sqrt583(const double& y) {  
    double x = 0.0, dx;  
  
    do {  
        dx = - (x*x-y) / (2.0*x);  
        x += dx;  
    } while (abs(dx) > 1.e-9);  
  
    return x;  
}
```

Const lvalue ref

- With following declarations:

```
double sqrt583(double x);
```

```
double sqrt583(double& x);
```

Temp x+y can be referenced if read only

```
double sqrt583(const double& x);
```

OK to reference const rvalue

I-values and r-values

- How is the value used in the function

```
double sqrt583(const double& y) {  
    double x = 0.0, dx;  
  
    do {  
        dx = - (x*x-y) / (2.0*x);  
        x += dx;  
    } while (abs(dx) > 1.e-9);  
  
    y = x;  
  
    return x;  
}
```

Const lvalue ref

```
$ c++ -c sl11.cpp  
error: cannot assign to variable 'y' with  
const-qualified type 'const double &'  
      y = x;  
      ~ ~  
sl11.cpp:3:30: note: variable 'y' declared const here  
double sqrt583(const double& y) {  
~~~~~  
1 error generated.
```

Reusing functions

```
#include <iostream>
#include <cmath>

double sqrt583(double z) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-z) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }

    return x;
}

int main () {

    std::cout << sqrt583(2.0) << std::endl;

    return 0;
}
```

```
$ c++ main.cpp
$ ./a.out
1.4142
```

Compile main.cpp

Translate it into a language the cpu can run

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

The executable (program that the cpu can run)

```
$ ./a.out
```

Reusing in other programs

```
#include <cmath>

double sqrt583(double& z) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-z) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }

    return x;
}
```

Put this function in its own file
amath583.cpp

Many programs (mains) can call it

```
#include <iostream>
#using namespace std;
int main () {

    cout << sqrt583(3.0) << endl;
    return 0;
}
```

```
#include <iostream>
#using namespace std;
int main () {

    cout << sqrt583(3.14) << endl;
    return 0;
}
```

```
#include <iostream>
#using namespace std;
int main () {

    cout << sqrt583(42.0) << endl;
    return 0;
}
```

Reusing in other programs

Many mains can call it

```
#include <iostream>
using namespace std;
int main () {

    cout << sqrt583(42.0) << endl;

    return 0;
}
```

Defined in a
different file

```
#include <cmath>

double sqrt583(double z) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-z) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }

    return x;
}
```

```
sqrt3.cpp:8:11: error: use of undeclared identifier 'sqrt583'
    cout << sqrt583(2.0) << endl;
               ^
sqrt3.cpp:9:11: error: use of undeclared identifier 'sqrt583'
    cout << sqrt583(3.0) << endl;
               ^
2 errors generated.
```

Undeclared
identifier

Didn't we declare
it here?

This is **definition**

Reusing functions

Doesn't know how to
translate this

```
#include <iostream>
using namespace std;
int main () {
    cout << sqrt583(42.0) << endl;
    return 0;
}
```

```
$ c++ main.cpp
$ ./a.out
1.4142
```

Compile main.cpp

Translate it into a
language the cpu can run

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

The executable (program
that the cpu can run)

```
$ ./a.out
```

Reusing functions across programs

Declare sqrt583 is a function that exists

~~clude~~ <iostream>

Returns a double

```
double sqrt583(double);  
  
int main () {  
    std::cout << sqrt583(42.0) << std::endl;  
  
    return 0;  
}
```

Takes a double

Now we know how to call it

Reusing in other programs

```
#include <iostream>

double sqrt583(double);

int main () {

    std::cout << sqrt583(42.0) << std::endl;

    return 0;
}
```

Many mains can call sqrt583

Undefined symbol

Linker command failed

```
Undefined symbols for architecture x86_64:
    "sqrt583(double const&)", referenced from:
        _main in sqrt3-1d1d35.o
ld: symbol(s) not found for architecture x86_64
clang: error: linker command failed with exit code 1 (use -v to see invocation)
```

Reusing functions

```
#include <iostream>

double sqrt583(double);

int main () {

    std::cout << sqrt583(42.0) << std::endl;

    return 0;
}
```

```
$ c++ main.cpp
$ ./a.out
1.4142
```

Compile main.cpp

Translate it into a language the cpu can run

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

The executable (program that the cpu can run)

```
$ ./a.out
```

Needs to find sqrt583 somewhere

Reusing in other programs

```
#include <iostream>
double sqrt583(const double& x);
```

Declare sqrt583

```
using namespace std;

int main () {
    cout << sqrt583(2.0) << endl;
    cout << sqrt583(3.0) << endl;

    return 0;
}
```

Undefined symbols for architecture x86_64:
 "sqrt583(double const&)", referenced from:
 _main in sqrt3-1d1d35.o
ld: symbol(s) not found for architecture x86_64
clang: **error:** linker command failed with exit code 1 (use -v to see invocation)

Reusing in other programs

```
#include <iostream>
using namespace std;
int main () {
    cout << sqrt583(42.0) << endl;
    return 0;
}
```

```
#include <cmath>

double sqrt583(double z) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-z) / (2.0*x);
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }

    return x;
}
```

\$ c++ main.cpp sqrt583.cpp

Compile main.cpp **with** sqrt583.cpp

Translate it into a language the cpu can run

The executable (program that the cpu can run)

\$./a.out

Reusing in other programs

```
#include <iostream>
using namespace std;
int main () {

    cout << sqrt583(42.0) << endl;

    return 0;
}
```

\$ c++ main.cpp

Compile main.cpp by itself

```
#include <cmath>

double sqrt583(double z) {
    double x = 1.0;

    for (size_t i = 0; i < 32; ++i) {
        double dx = - (x*x-z) / (2.0*x) ;
        x += dx;
        if (abs(dx) < 1.e-9) break;
    }

    return x;
}
```

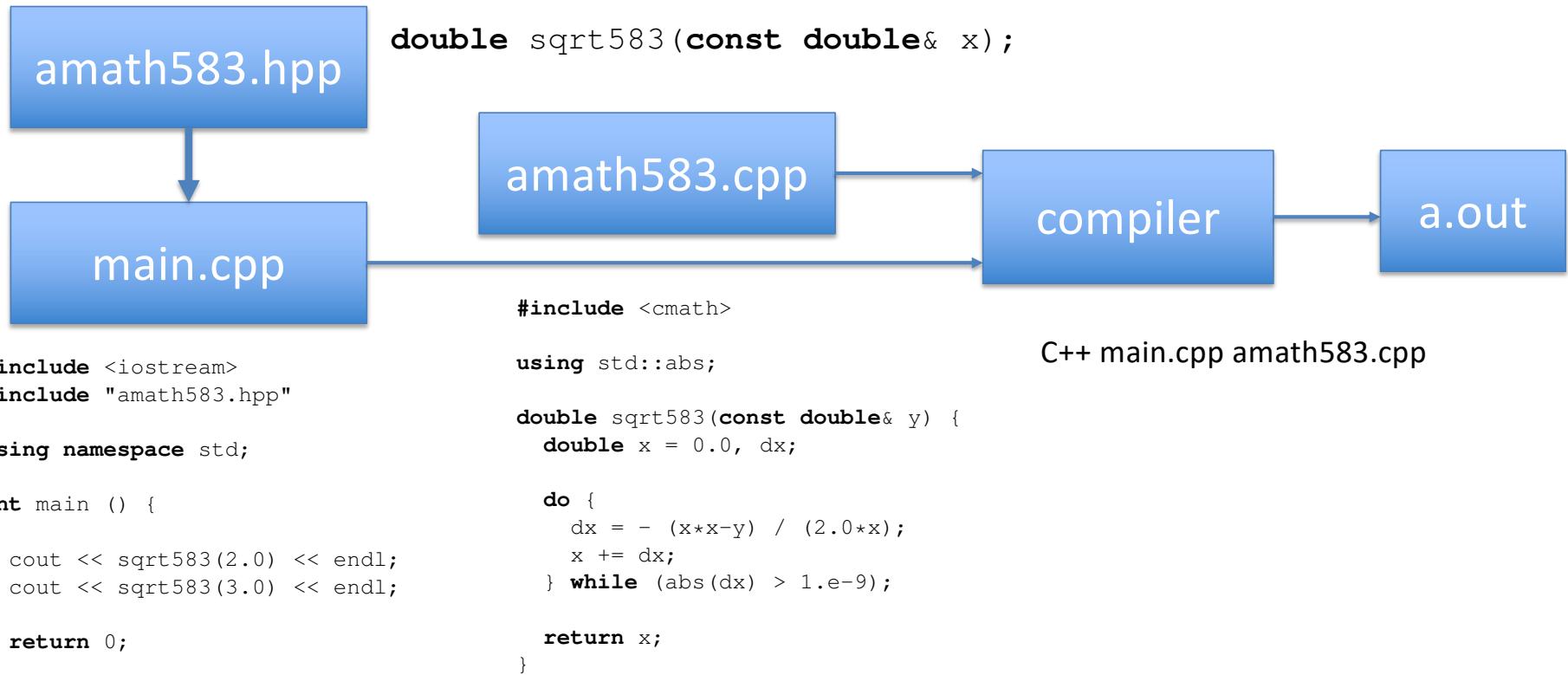
\$ c++ sqrt583.cpp

Compile sqrt583.cpp by itself

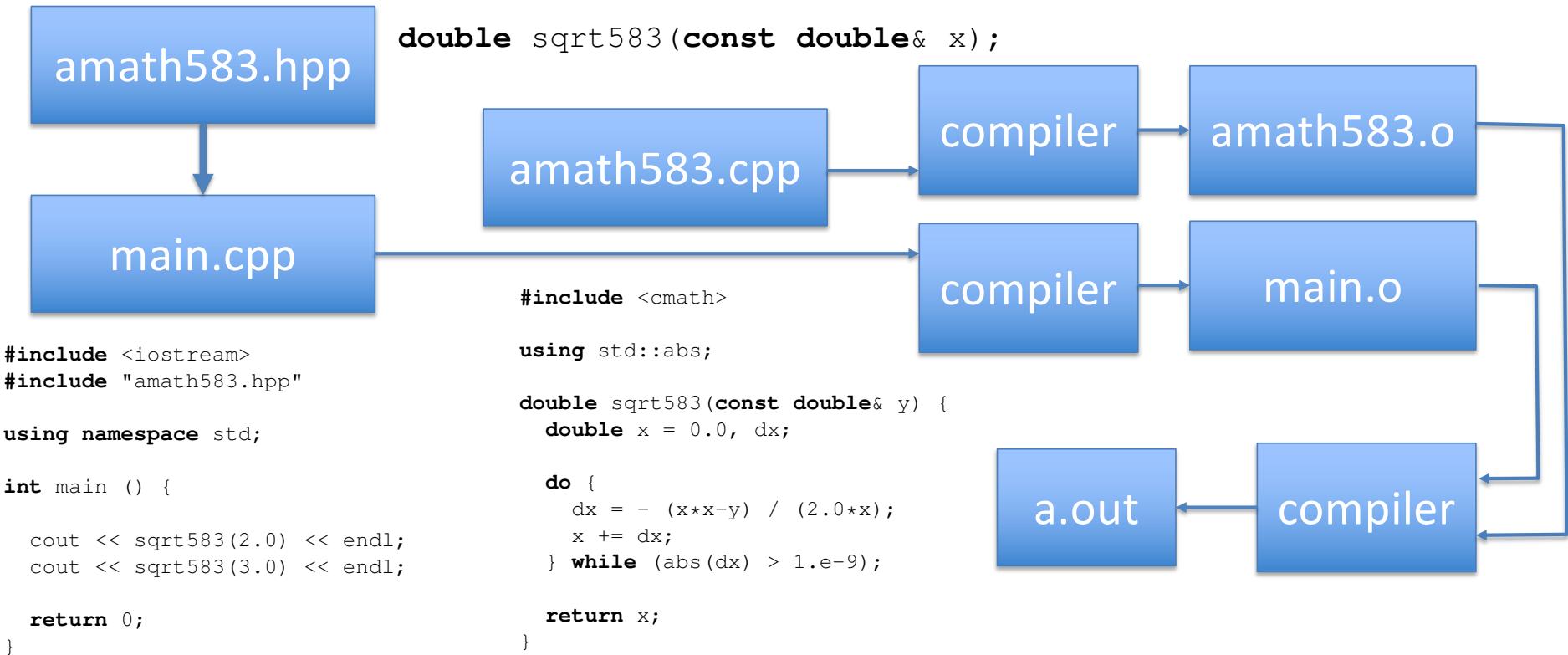
\$./a.out

Generate executable

One more refinement in organization



One more refinement in organization



Multifile Multistage Compilation

Compile main.cpp to
main.o object file

Tell the compiler to
generate object

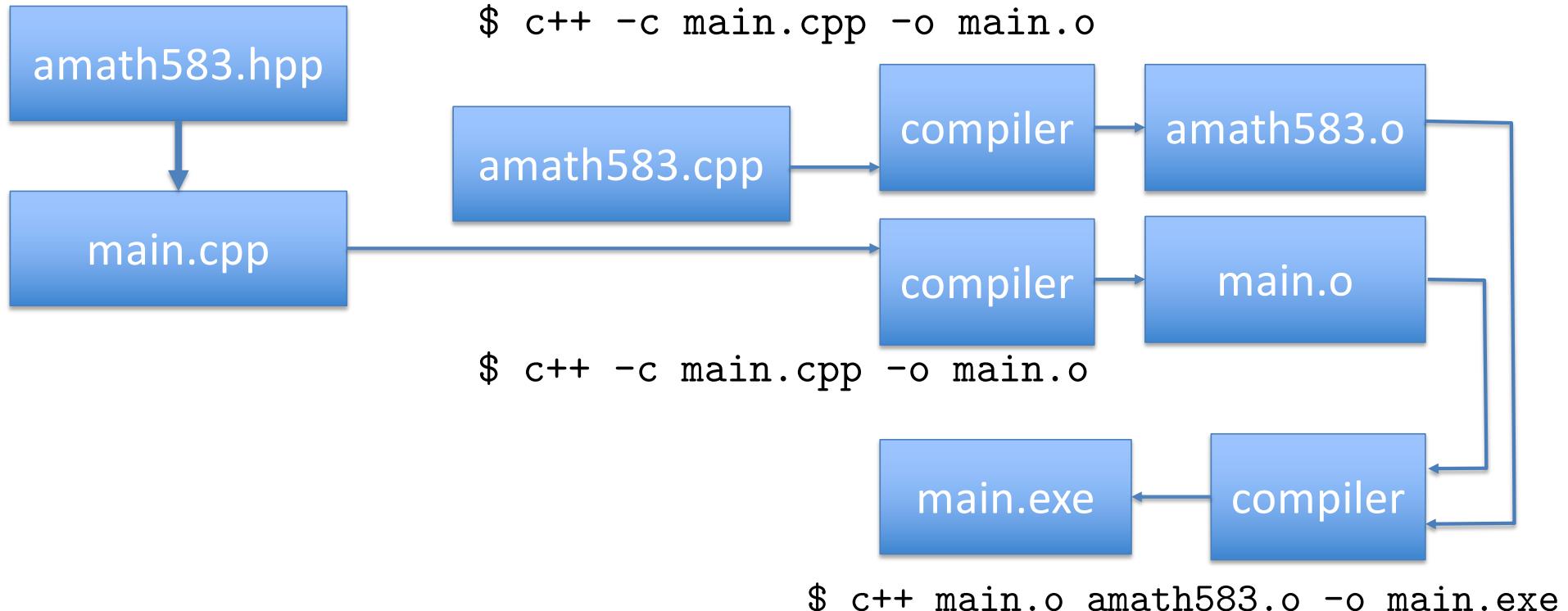
```
$ c++ -c main.cpp -o main.o
```

Tell the compiler
name of the object

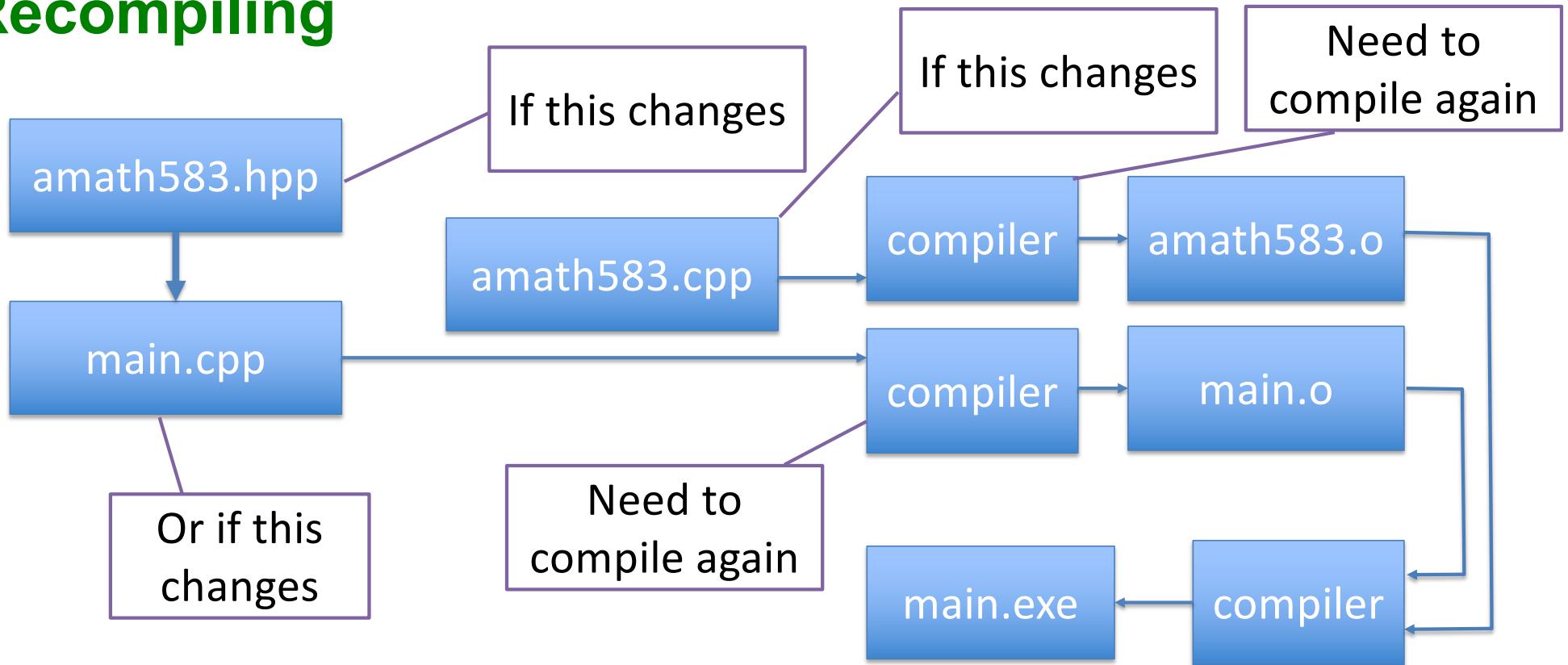
```
$ c++ -c amath583.cpp -o amath583.o
```

```
$ c++ main.o amath583.o -o main.exe
```

One more refinement in organization



Recompiling



Dependencies

- main.o depends on main.cpp and amath583.hpp
- amath583.o depends on amath583.cpp
- main.exe depends on amath583.o and main.o



Automating: The Rules

- If main.o is newer than main.exe → recompile main.exe
- If amath583.o is newer than main.exe → recompile main.exe
- If main.cpp is newer than main.o → recompile main.o
- If amath583.cpp is newer than amath583.o → recompile amath583.o
- If amath583.hpp is newer than main.o → recompile main.o

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AMATH 483/583 High-Performance Scientific Computing Spring 2019
University of Washington by Andrew Lumsdaine

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Make

- Tool for automating compilation (or any other rule-driven tasks)
- Rules are specified in a makefile (usually named “Makefile”)
- Rules include
 - Dependency
 - Target
 - Consequent

Target

```
main.exe: main.o amath583.o  
        c++ main.o amath583.o -o main.exe  
  
main.o: main.cpp amath583.hpp  
        c++ -c main.cpp -o main.o  
  
amath583.o: amath583.cpp  
        c++ -c amath583.cpp -o amath583.o
```

Dependencies

Consequent

Make

- Tool for automating compilation (or any other rule-driven tasks)
- Rules are specified in a makefile (usually named “Makefile”)
- Rules include
 - Dependency
 - Target
 - Consequent
- Edit amath583.hpp

```
$ make
c++ -c main.cpp -o main.o
c++ -c amath583.cpp -o amath583.o
c++ main.o amath583.o -o main.exe
```

```
$ make
c++ -c main.cpp -o main.o
c++ main.o amath583.o -o main.exe
```

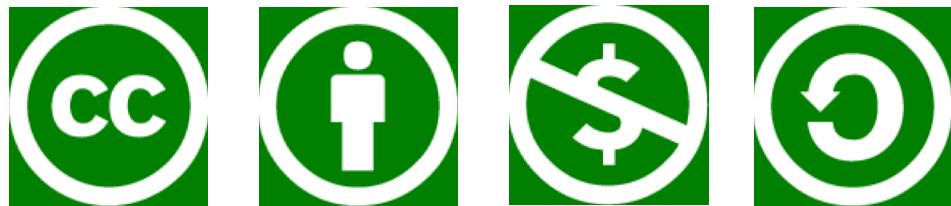
Thank you!

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