Lecture 03 – Programming Languages ~~and Scripting~~

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NERS/ENGR 570 - Methods and Practice of Scientific Computing (F20)

COLLEGE OF ENGINEERING
NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
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Outline

- Survey Results
- C and C++ with comparison to Fortran
- Resuming hands on from last lecture
  - Review Fortran code, write C and C++ examples
- ~~Introduction to Bash Scripting (time permitting)~~

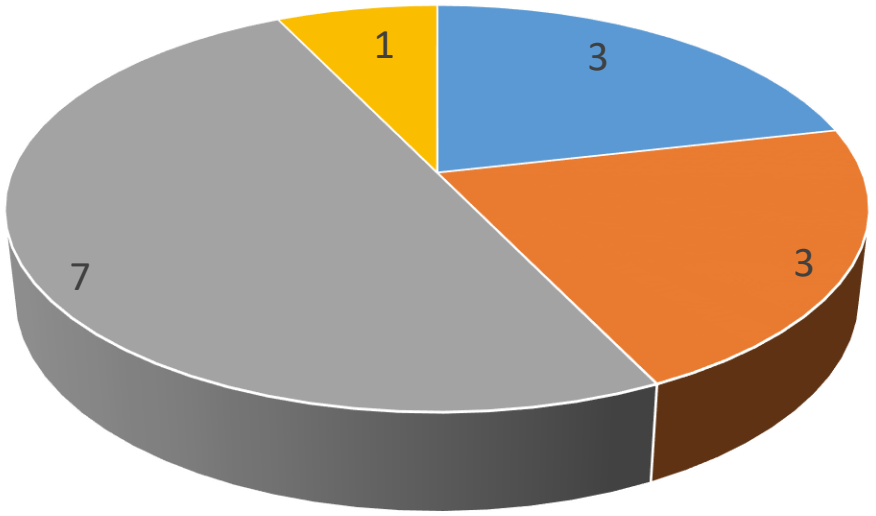
Learning Objectives: By the end of Today's Lecture you should be able to

- *(Knowledge)* clearly understand what we'll be teaching the rest of the semester and the overall previous experience of the class
- *(Skill)* Declare variables that are matrices, and assign or edit their values in Fortran, **C, and C++**
- *(Knowledge)* describe relationships between some language aspects of C/C++ with respect to Fortran
- ~~*(Knowledge)* avoid simple syntax mistakes in Bash~~

Survey Results

Participation

Format



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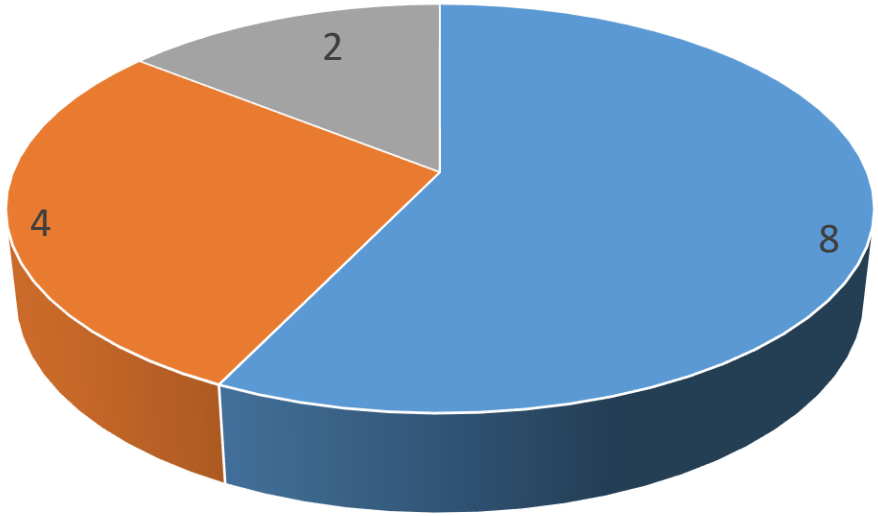

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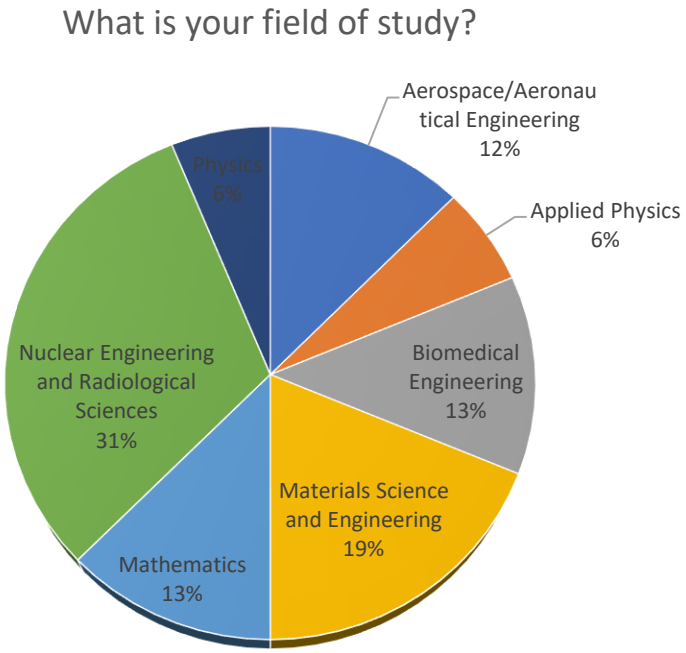

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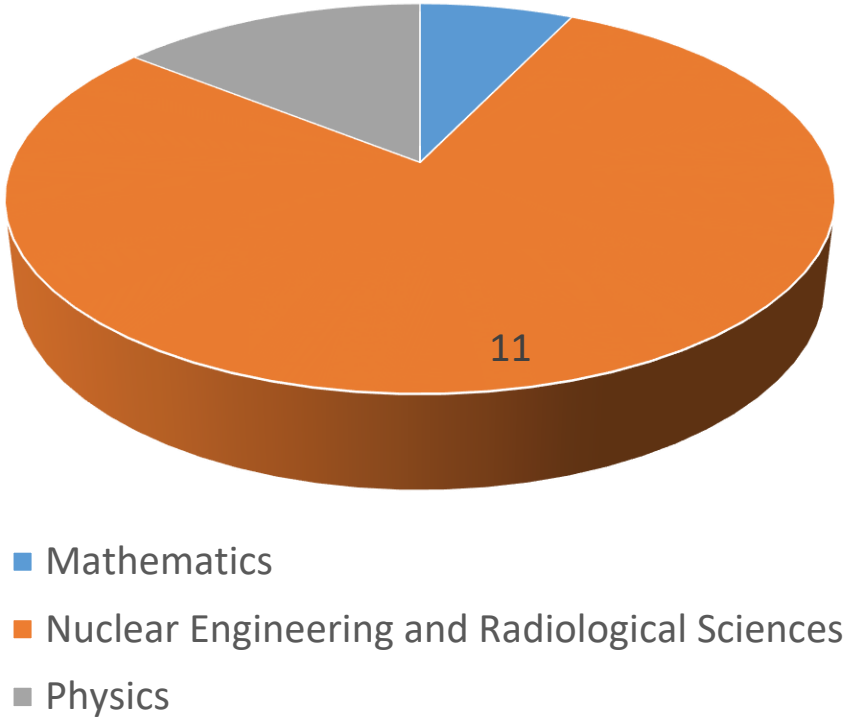

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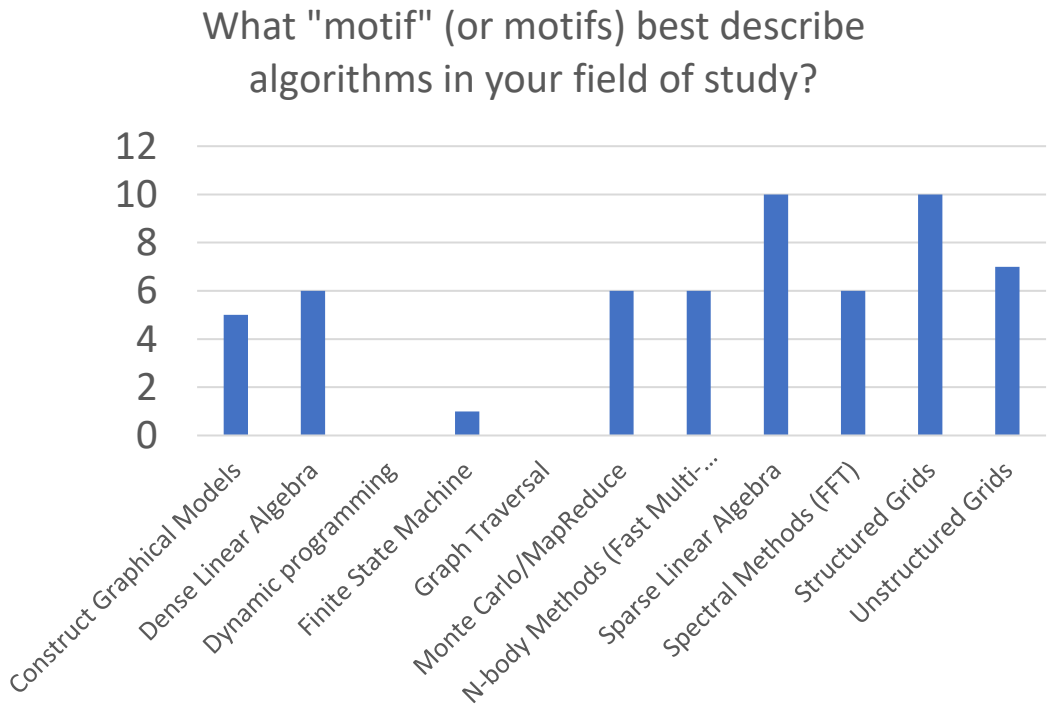

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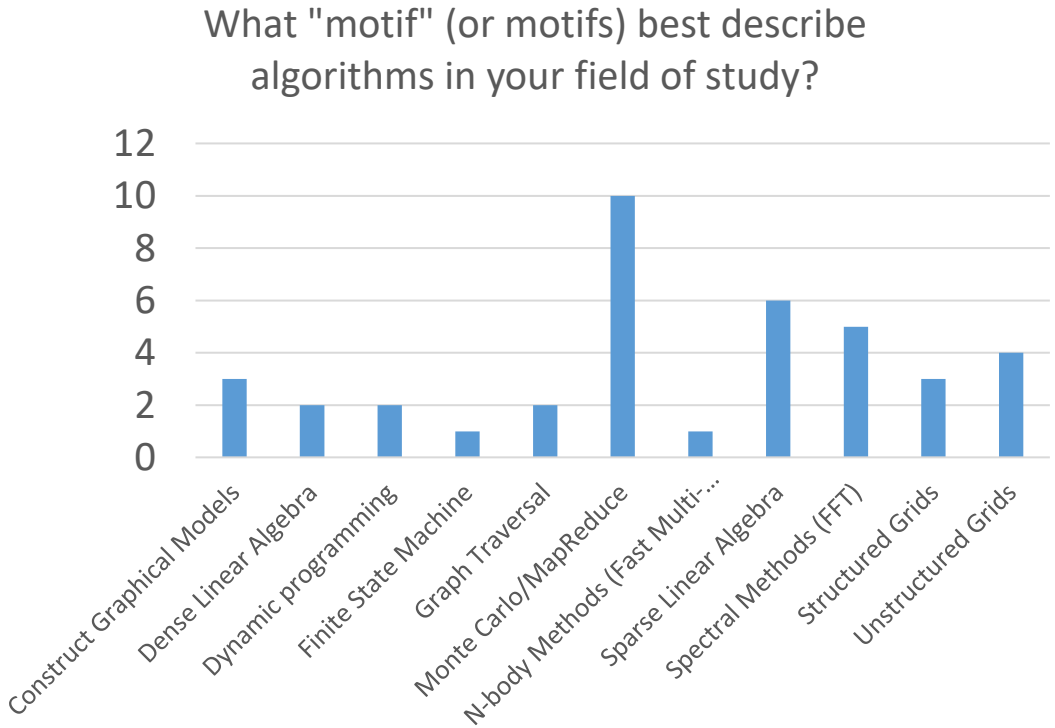

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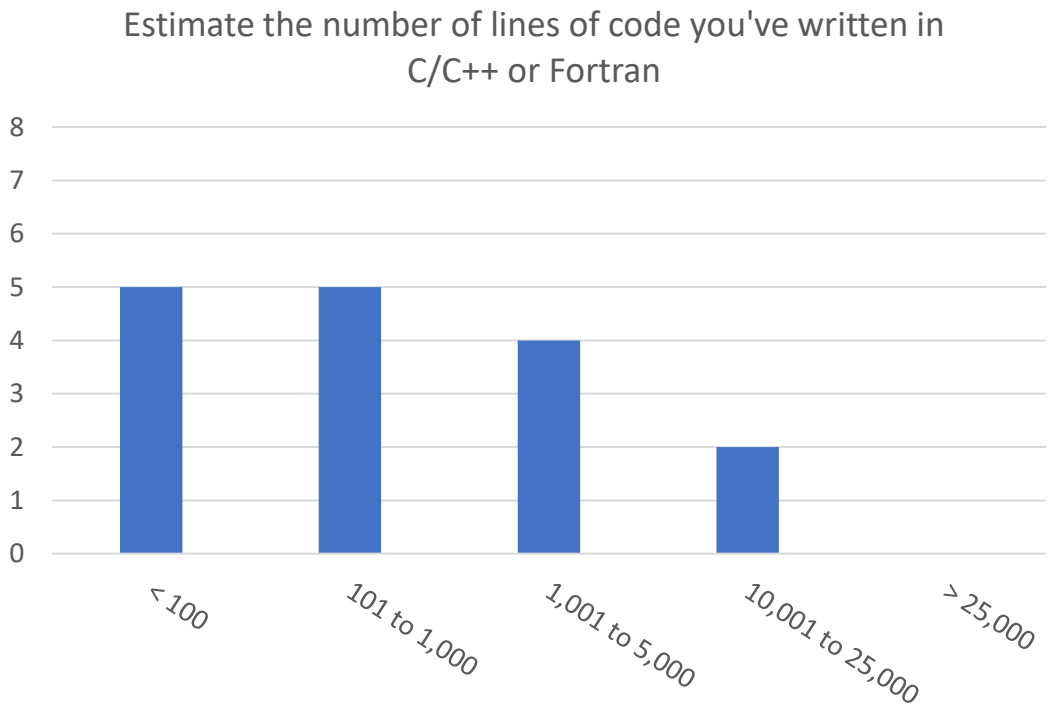

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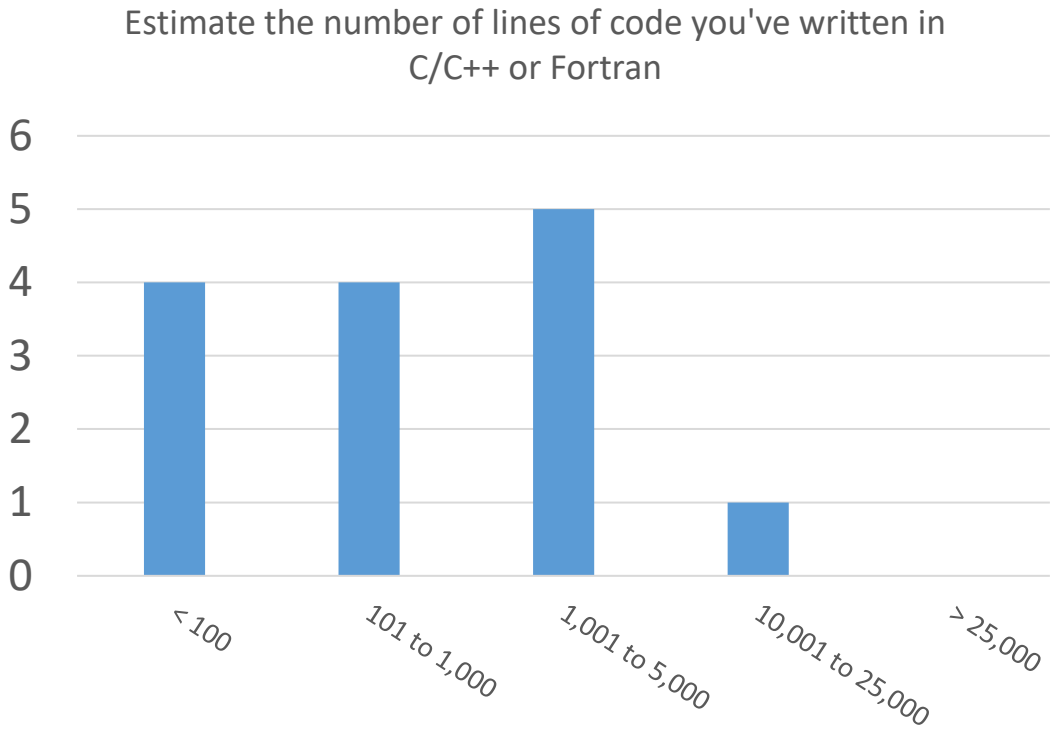

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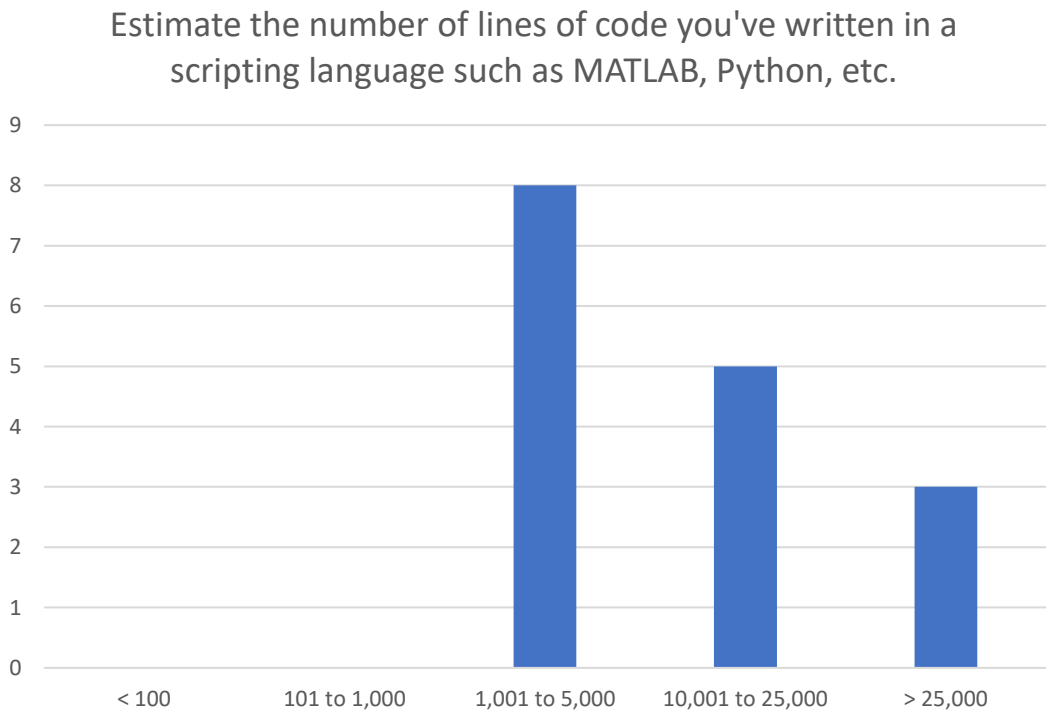

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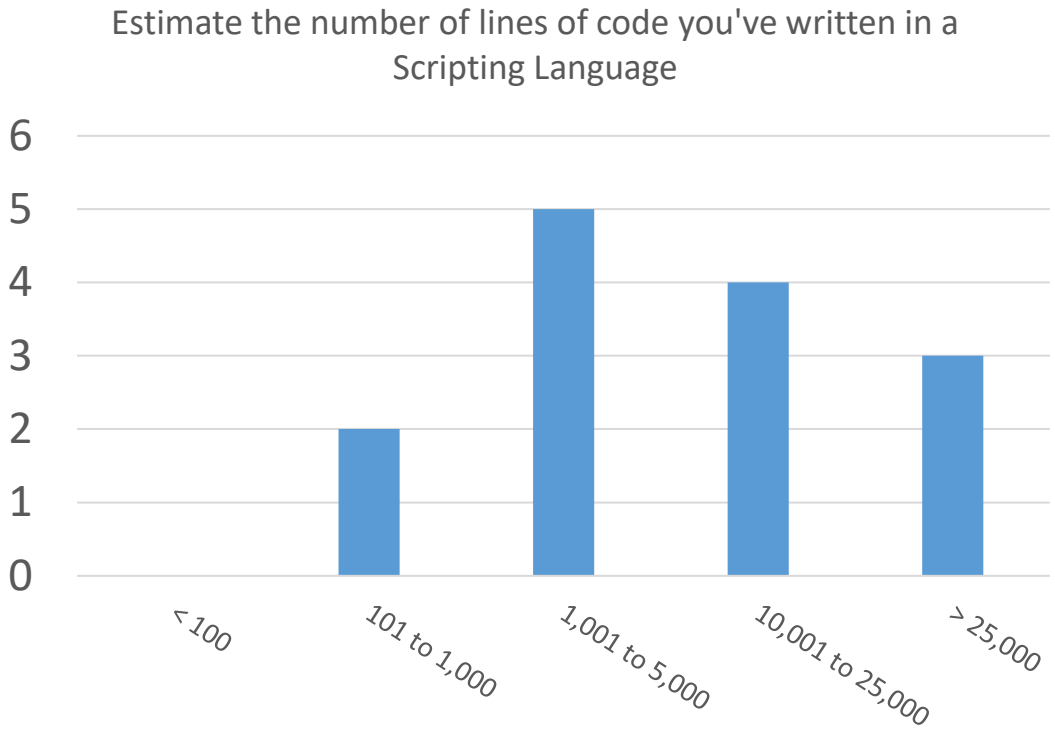

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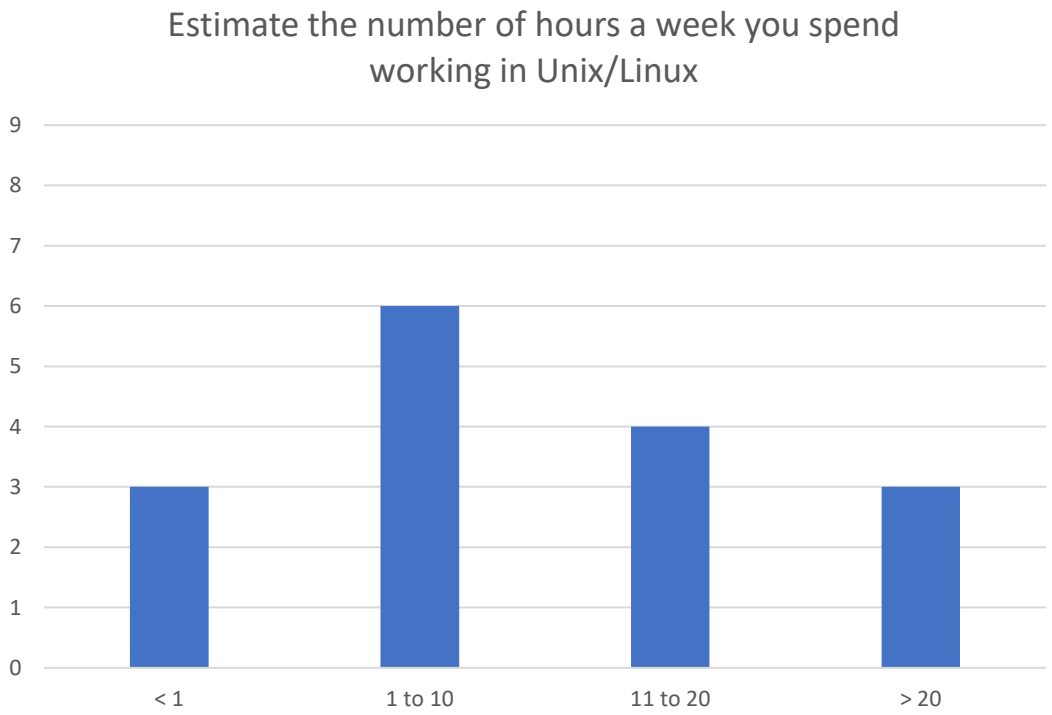

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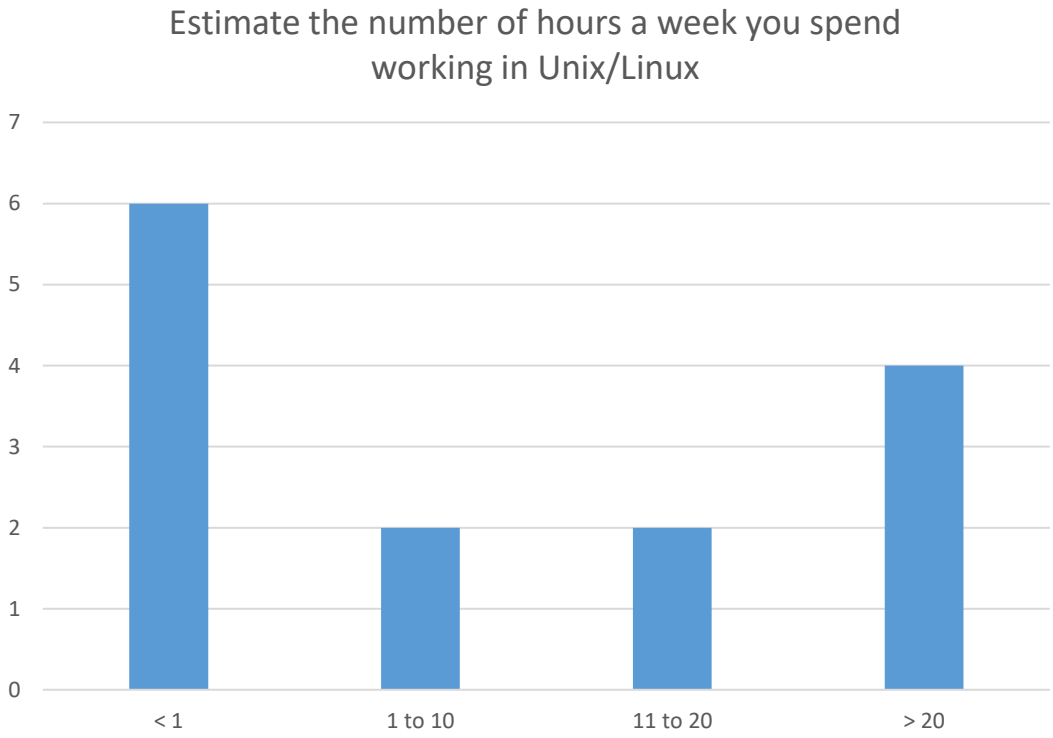

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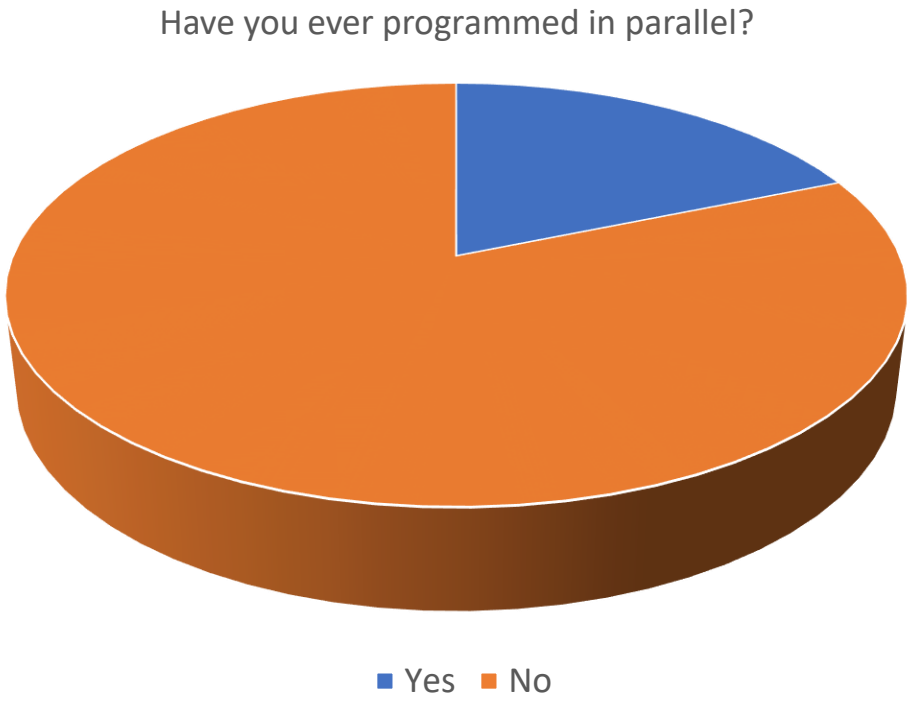

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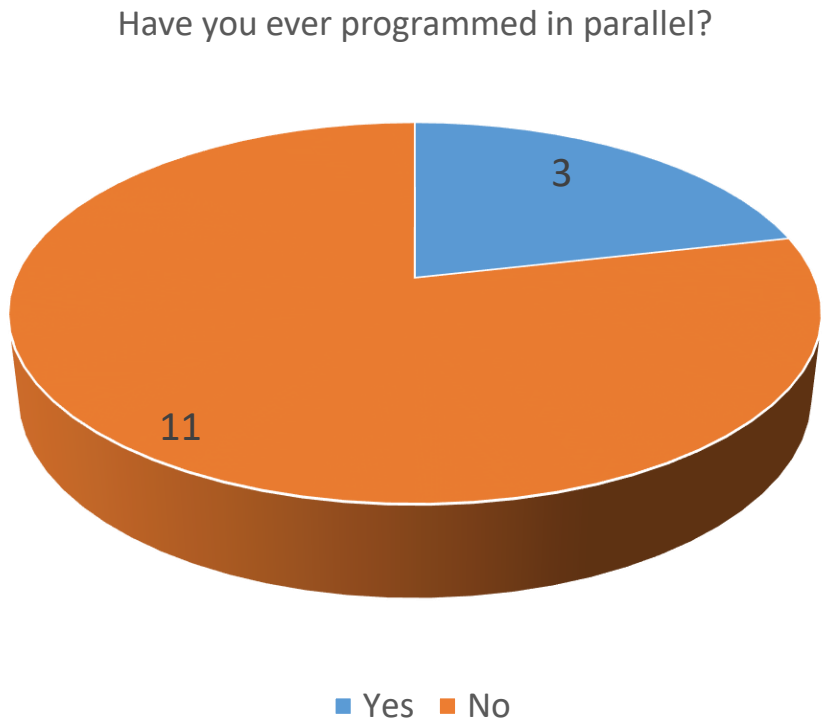

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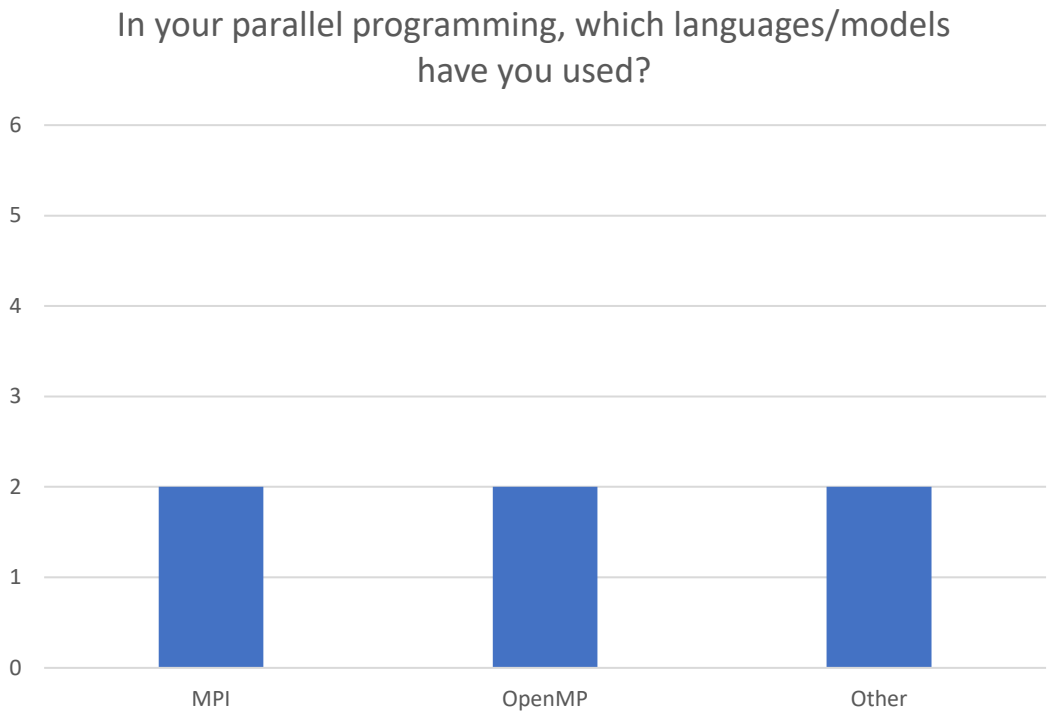

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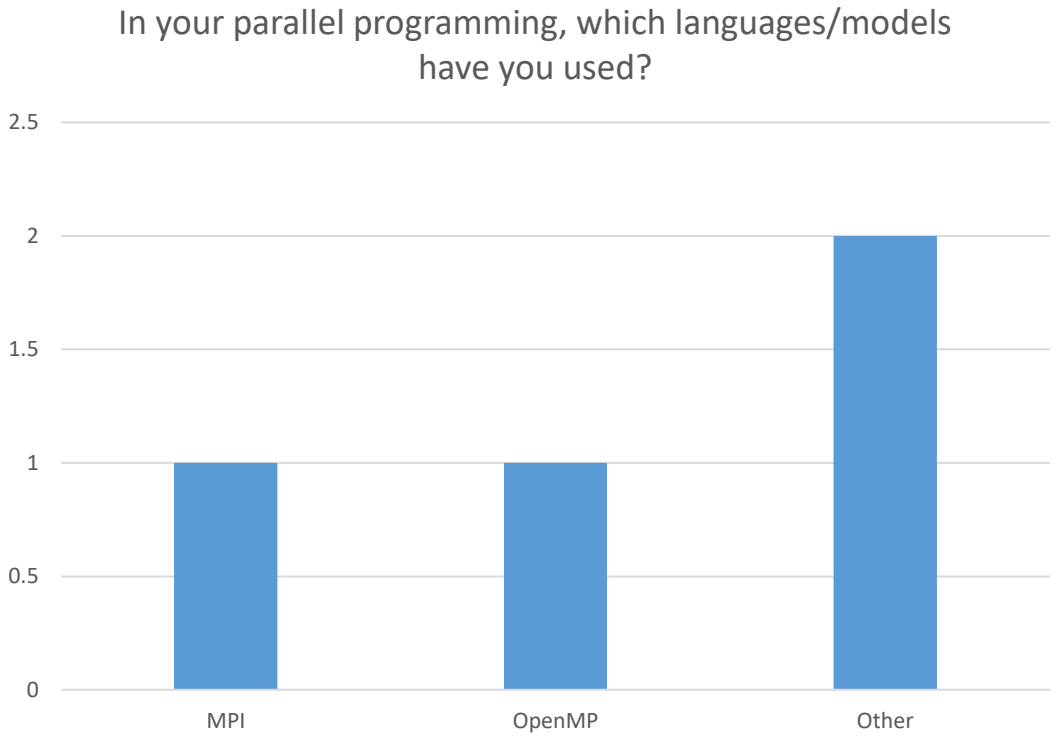

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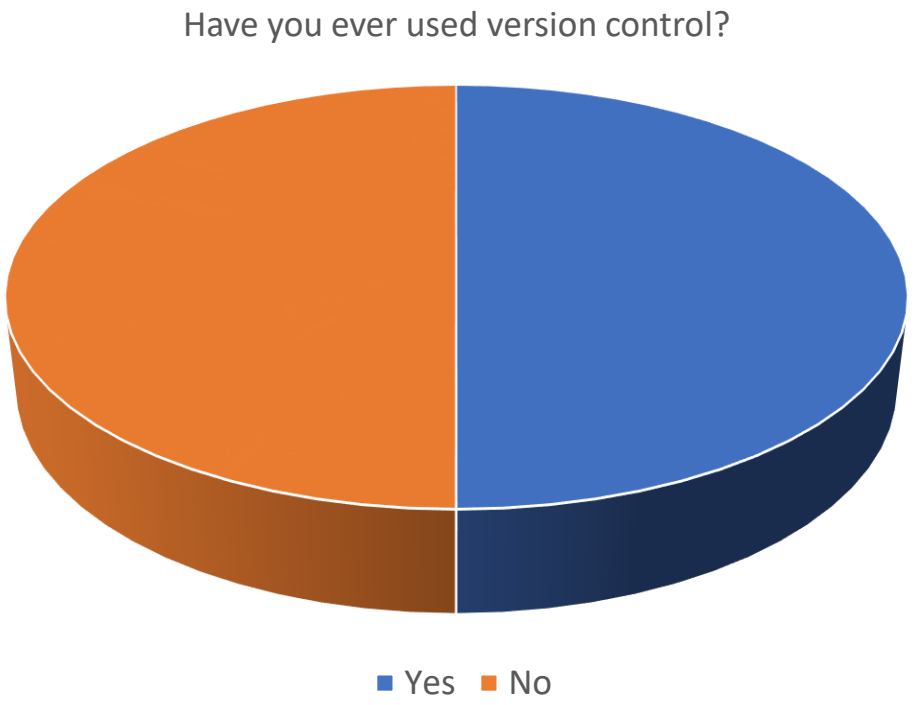

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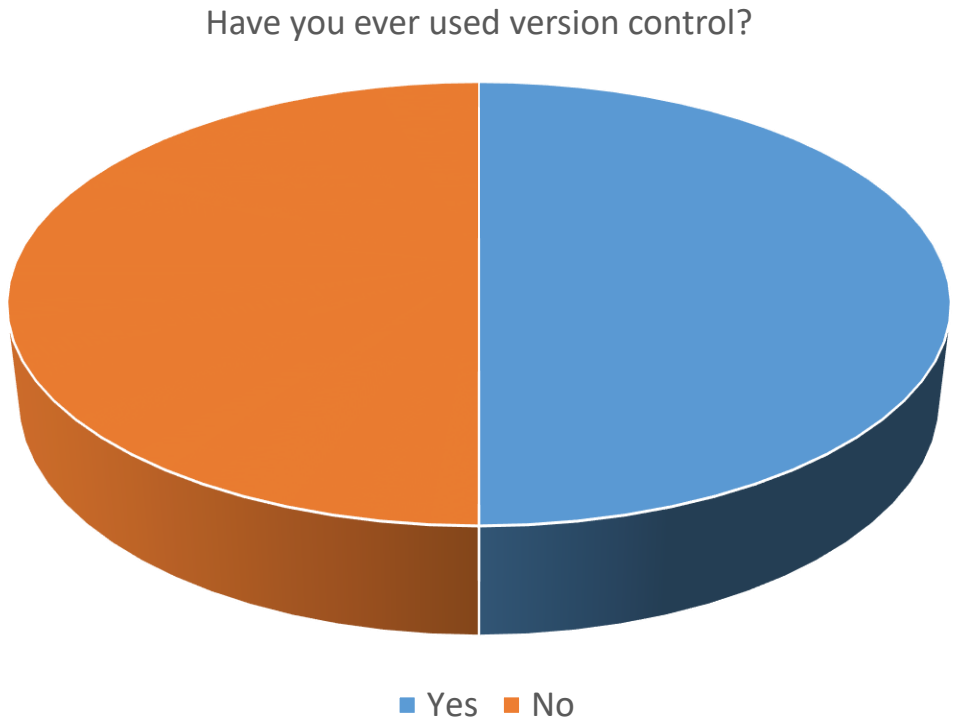

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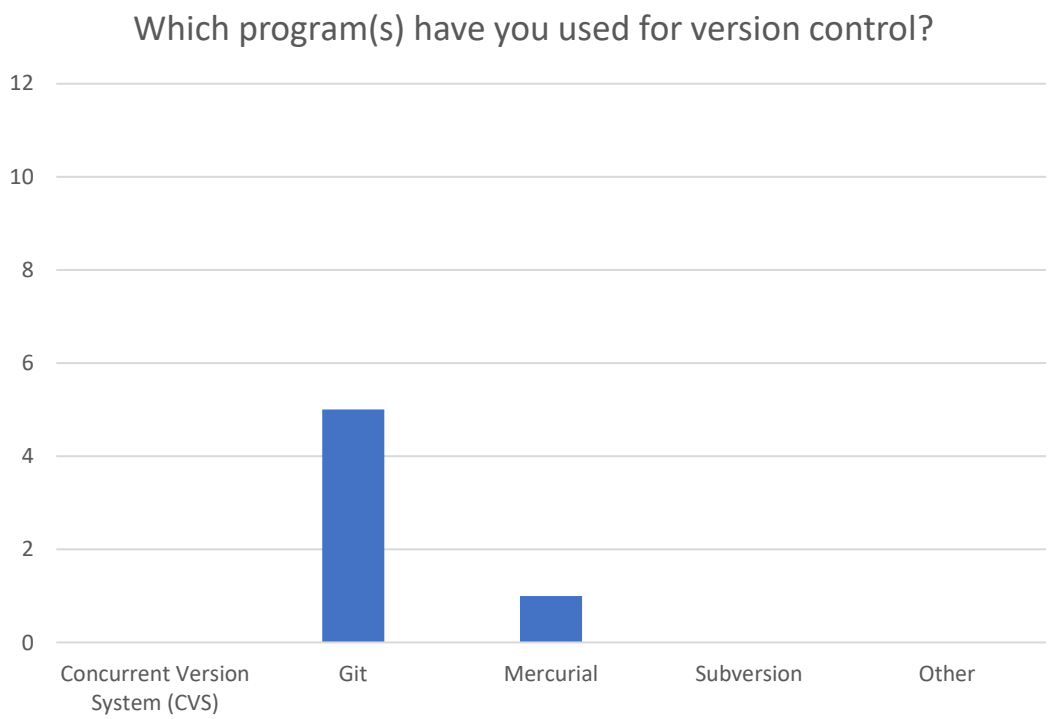

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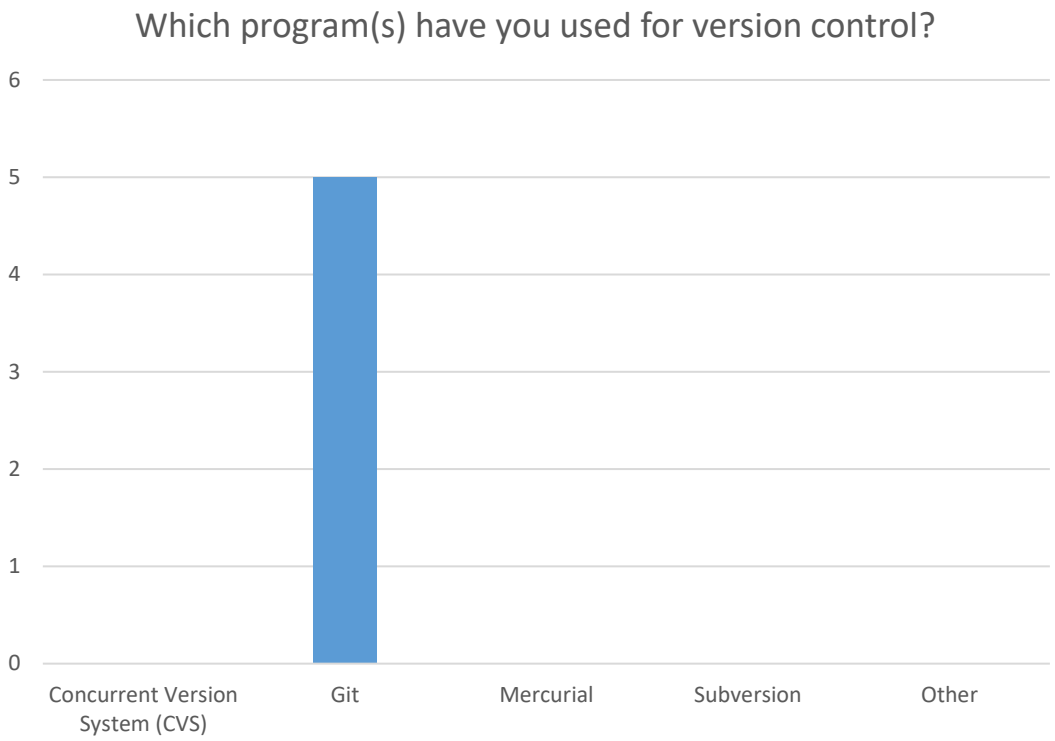

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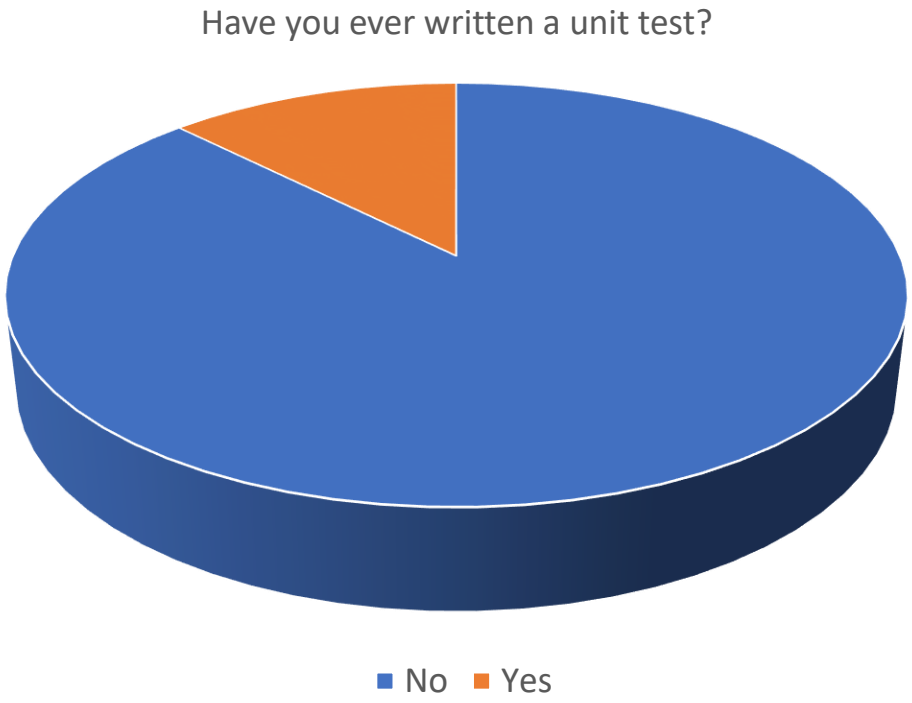

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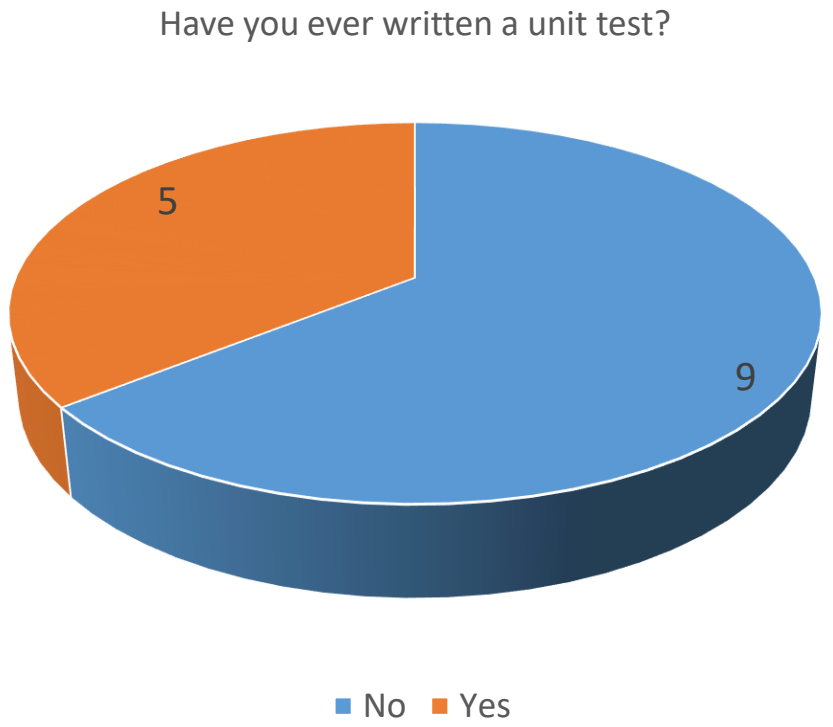

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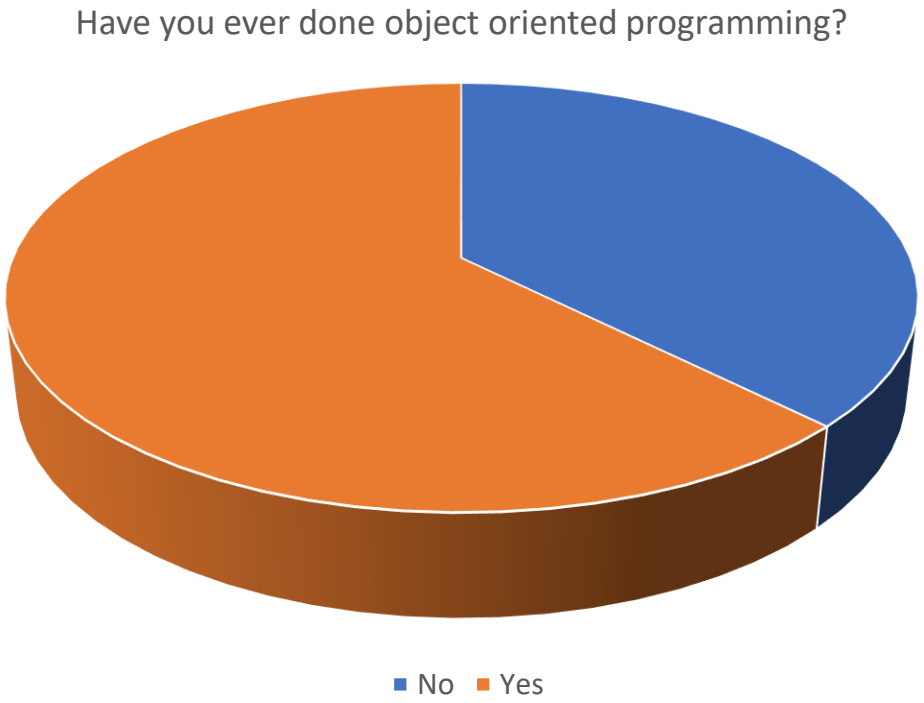

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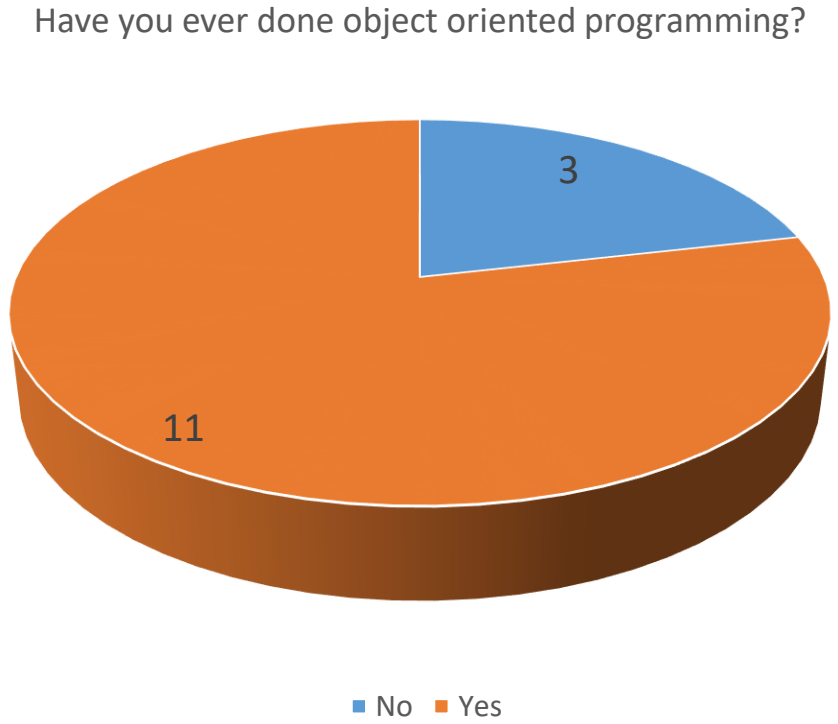

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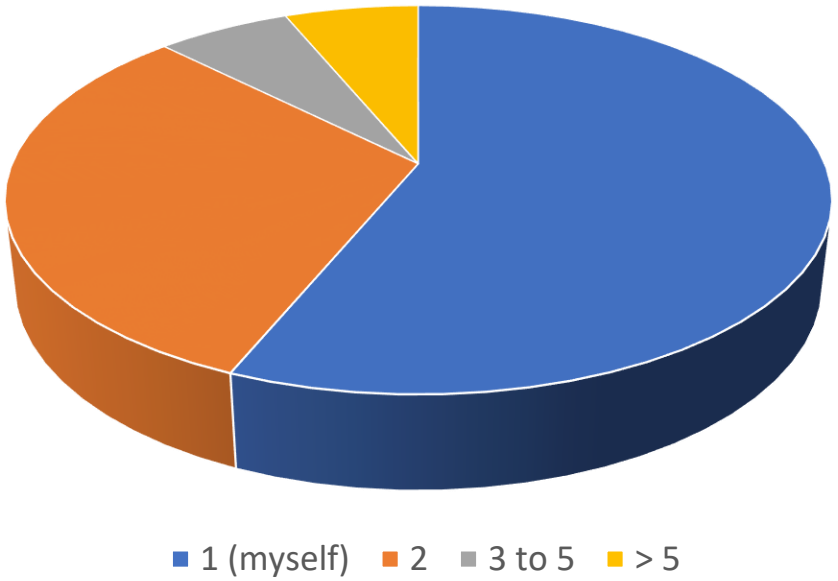

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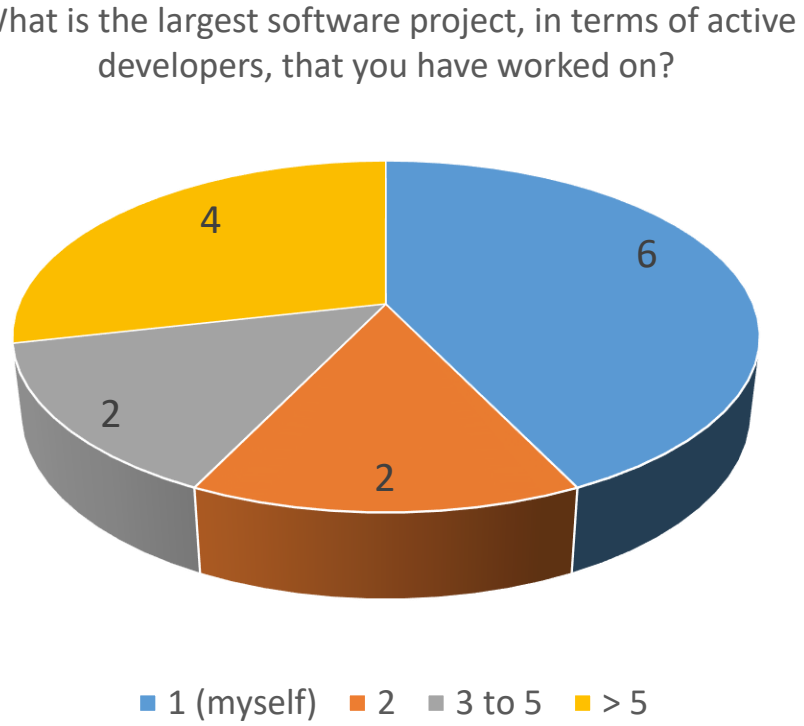

Are You already working with software in your research?

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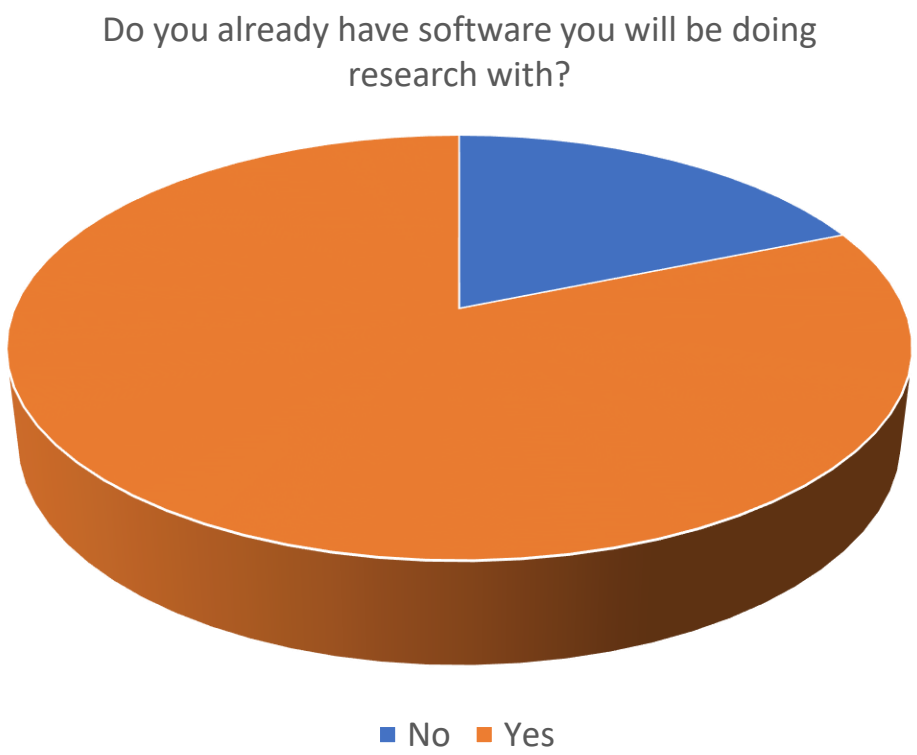

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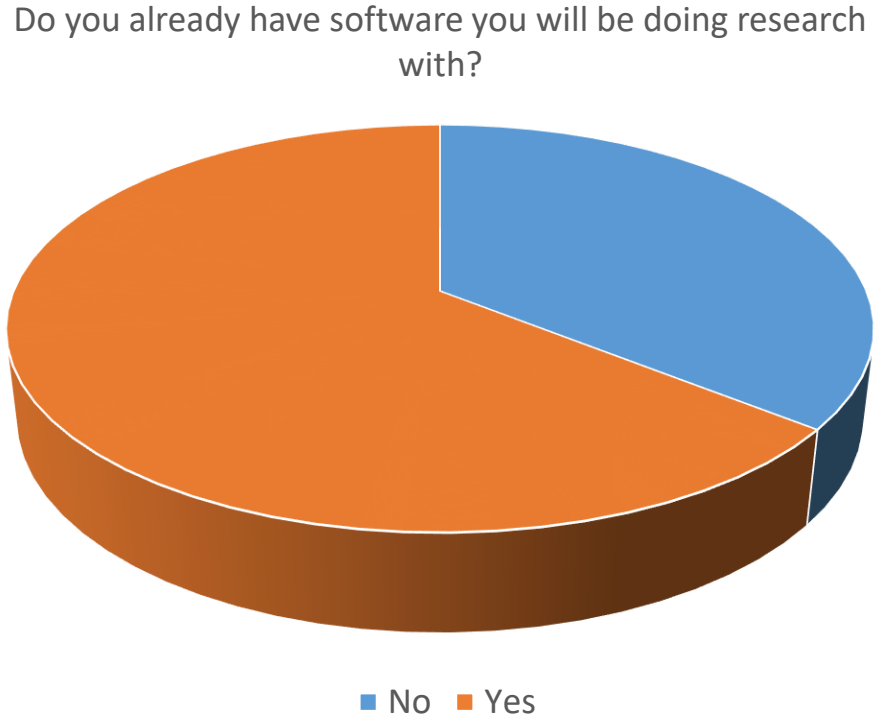

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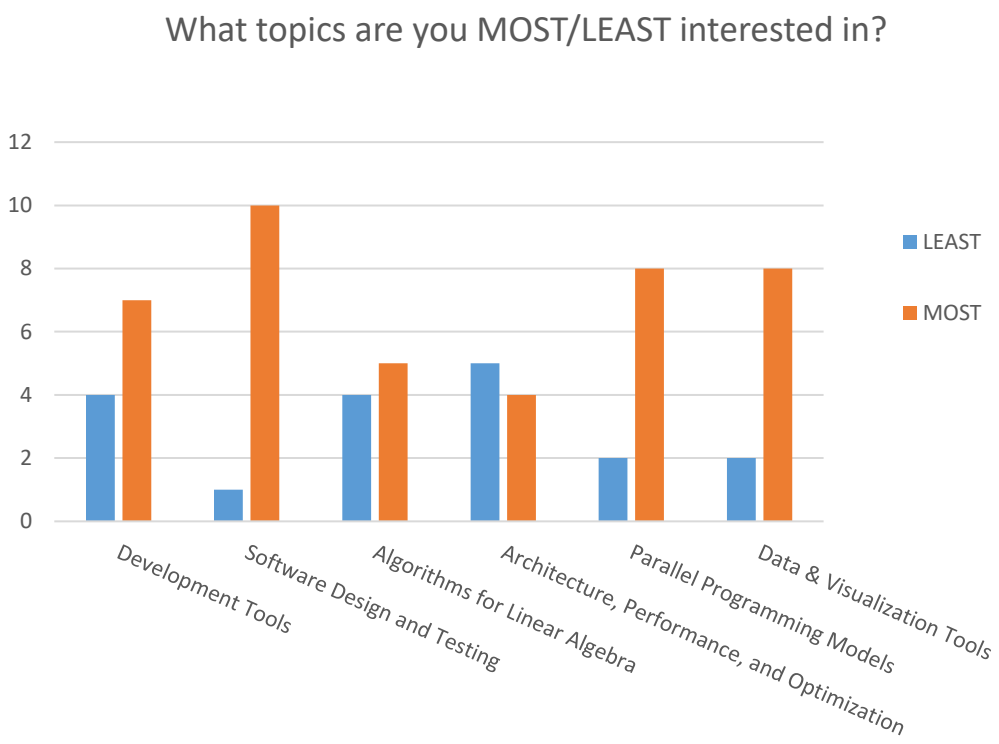


- What other topics?
  - Machine Learning
  - GPUs
  - Pair Programming
  - Portability
  - Working on an HPC

What do I want out of this course?

2019

- Work more efficiently
  - Efficient workflow
  - Write code more efficiently
  - Write faster code
  - Spend less time debugging
- Improve Programming Skills
- Working on large projects

2020

- Use HPC
- Become a better/more efficient programmer
- Become more aware of tools
- Work on large projects

Programming Languages

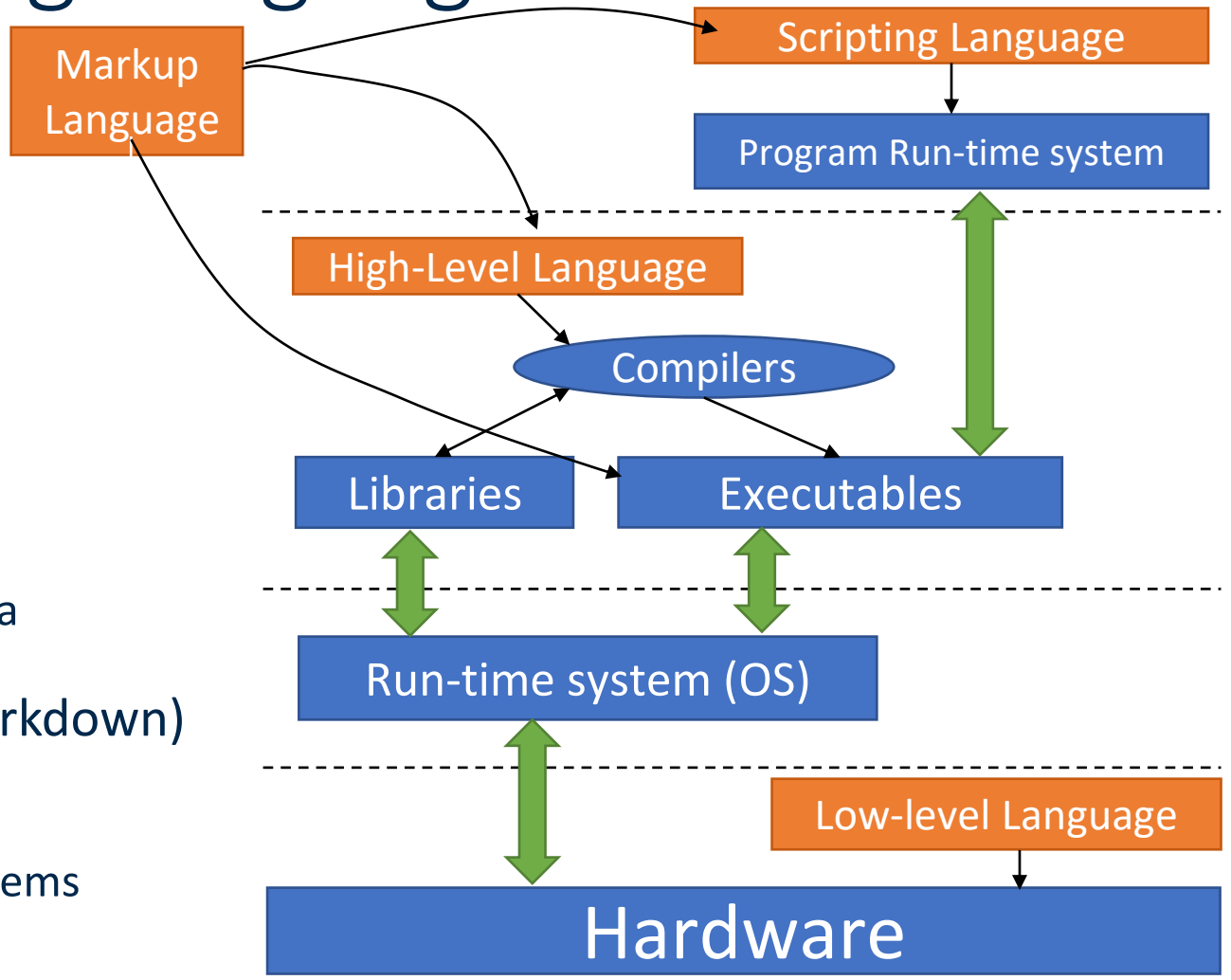
Recap

What defines a programming language?

- Primarily: A formal standard
  - C/C++: C89, C99, C11 and C++98, C++03, C++11, C++14, C++17
  - Fortran: ISO/IEC standard 1539
  - Java
  - Python
- Syntax: e.g. the “grammar”
- Semantics: e.g. the “meaning” which is “vocabulary + grammar”
- Programming languages should define performance of execution
  - Typically syntax/semantics are carefully defined, but not so for performance model.

Types of Programming Languages

- Low Level language (Assembly)
  - Defined by hardware (less portable)
- High Level language (C/C++, Fortran, Java)
  - Defined by run-time system (e.g. Operating System)
  - Portable, depends on compilers
- Scripting language (MATLAB, Python, Bash)
  - Defined by portable run-time system of a program
- Markup language (e.g. XML, YAML, Markdown)
  - Used for annotation
  - Data transfer
  - Input to multiple types of programs/systems



Things a programming language should do

- Variable declaration
  - Scalars, arrays, pointers
  - Intrinsic types, programmer defined types
- Operators
  - Arithmetic: +, -, *, /
  - Relational: <, >, ==
  - Logical: and, or, not, xor
  - Others: e.g. exponentiation
- Execution control constructs
  - Branching constructs
    - e.g. if/else, switch (or case)
  - Looping constructs
    - For or Do
    - While
  - Goto
- Memory management
  - Automatic
  - Or provide programmer with intrinsics

Fortran Recap

Fortran 90/95

- F90 Standard: ISO/IEC standard 1539:1991
- F95 Standard: ISO/IEC 1539-1:1997
- Free Form
  - Forget all the rules about columns
- Dynamic memory allocation
- Intrinsic support for array operations
  - (e.g. a(:)=b(:))
- Pointers: references to memory
- Modules: reusable components of program
- Derived data types: custom data types
- Removed some problematic features of F77

```
module linear_system
  type :: linsys_t
    real,pointer :: a(:,:),b(:),x(:)
  end type

  integer :: n
end module
```

```
program main
use linear_system
implicit none

real,pointer :: sol(:)
type(linsys_t) :: ls1,ls2

read(*,*) n
allocate(ls1%a(n,n))
allocate(ls1%b(n))
allocate(sol(n))
ls1%x => sol
! ...
```

Fortran 2003 & 2008

Fortran 2003: ISO/IEC 1539-1:2004

- Significant addition to F90/95
  - F90/95 programs are F2003 compliant
- Defined Object-Oriented Features
  - Polymorphism and inheritance
  - Type-bound procedures (methods)
- Other
  - Procedure pointers
  - Standardized C-interoperability
  - IEEE floating point arithmetic
  - Enhanced intrinsics for command line processing

Fortran 2008: ISO/IEC 1539-1:2010

- Primarily added language features for enhanced parallelism
- Added submodules
  - Entity facilitating program structure
- Coarray Fortran
  - Simple extension for distributed parallel programming
  - Typically relies on underlying MPI implementation
- DO CONCURRENT
  - Loop iterations have no interdependencies

C and C++

History of C/C++

- C - started in 1969 by Dennis Ritchie at Bell Labs
  - Concurrent with and related to the *development of Unix operating system* (also at Bell Labs)
  - Most widely used programming language – *available across virtually all platforms and architectures*
  - Informal specification "K&R" (Kernighan and Ritchie, the developers) published in 1978
  - ANSI standard since 1989
  - General purpose
  - Relatively fast
  - Current standard is C18
- C++ - also developed at Bell Labs, starting in 1979
  - Standardized in 1998 (International Organization for Standardization)
  - Added features/extensions that make development and management of large software projects much simpler (mainly classes)
  - Newer versions have more advanced functionality (templates, namespaces, abstract classes, and more)
  - Widely used for scientific computing purposes because of powerful Object-Oriented programming capabilities

C and C++ standards

C Standards

- C89
  - original ANSI standard (also C90)
  - still supported by compilers
- C99
  - new features include
    - function inlining,
    - `complex` type,
    - one-line comments with "`//`",
    - variable-length arrays, and more
- C11
  - atomic operations,
  - multi-threading,
  - bounds-checked functions,
  - static assertions
- C18
  - Revision to C11

C++ Standards

- C++98
  - First standard, introduces object-oriented features to C
    - Abstraction, Encapsulation, Inheritance, Polymorphism
  - ***Multiple inheritance***
- C++03
  - Mostly fixed issues with previous standard to improve compiler consistency
- C++11
  - Multi-threading, initializer lists for all classes, type inference (`auto`)
- C++14
  - ***Variable templates***, `deprecated` (for multi-threading), bug fixes, other
- C++17
  - No longer experimental in GNU compilers as of last month

Data Types

- Intrinsic – basic data types that are defined and recognized by standard C
  - Also available as multi-dimensional arrays
- Derived – library or user-defined data type that is made up of some combination of data with intrinsic types
  - Standard library: vector (of any data type), string
  - User-defined: a struct or class that contains several variables of any combination of intrinsic and/or derived types

Intrinsic Data Types	
Keyword	Details
`unsigned char`	8-bit integer 0 to 255
`signed char`	8-bit integer -127 to 128
`unsigned int`	`short` (16-bit), `long` (32-bit or 64-bit), and `long long` (64-bit)
`signed int`	
`float`	32-bit
`double`	64-bit
`complex` (C99)	`complex float` and `complex double`
`bool`	True or False
`enum`	enumeration for a set

Definable (Derived) Data Types	
Keyword	Details
`union`	Define several variables to share same memory space
`struct`	Defined in terms of intrinsic data types (or other `structs`)

C/C++ Variable Declaration

- In C/C++, legal variable declarations can be made *at any point within a code*
  - Unlike Fortran, where all type declarations are made at the top of a routine or program
  - For C90, must be immediately after {
- All variables must be declared as a certain type (and should be initialized) before being used in some expression
- Variables remain defined throughout the scope in which they were declared. When a variable "falls out" of scope, its data is no longer accessible
- Scope is defined in C++ by opening and closing curly braces {}

```
float variable;
int variable = value;
```

C Operators & Special Characters

Logical Operators	
&&	and
||	or
!	not

Arithmetic Operators	
+	addition
-	subtraction
*	multiplication
/	division
%	modulus
=	assignment

Other	
Symbol(s)	Meaning
// or /* */	Comment and comment block
;	End of statement
{ }	Scope declaration
? :	Ternary operator (like a compacted if/else)
[ ]	Array declaration
*	Dereference variable (Unary)
&	Return memory address of variable (Unary)
-> or .	Member selection (-> is for pointers, . is for non-pointers)

Relational Operators	
==	Equal to
!=	Not equal to
>	Greater than
>=	Greater than or equal to
<	Less than
<=	Less than or equal to

Augmented Assignment	
++	a=a+1
--	a=a-1
+=	a=a+b
-=	a=a-b
*=	a=a*b
/=	a=a/b

Bitwise Operators	
&	Bitwise AND
|	Bitwise OR
^	Exclusive OR
~	Toggle (flip) bits
>>	Left Shift
<<	Right Shift

Augmented assignment operators also available for bitwise operations

Program Entity Structure

Preprocessor statements (Header file declarations)

Global Declarations

In C++ Class declarations go here (will cover examples in more detail with OO programming)

Main program (only define once in program)

Functions

Other functions (optional)

```c
/* Preprocessor commands
   and include statements */
#include <stdio.h>

//Global variables and interface definitions
int n;
void sub1(int* n);

/* Functions/Subroutines
   "main" is a special procedure
   in C/C++ corresponding to the
   "main program" */
int main()
{
    sub1(&n);
    return n;
}
/* "void" means return nothing, like a Fortran
   subroutine */
void sub1(int *n)
{
  *n=0;
}
```

C example

Header Files

- Header files are used to define variables and interfaces
  - Generally each source file has a corresponding header file, especially in C++
- The header data is appended to the top of the source code files by the compiler when an #include "header.h" statement is present.
- Header files allow compilers to "resolve dependencies" in your program.
- In C++ header files:
  - Variables are declared not only as a specific type but also public or private
    - Public: any function has access to read, use, and change this data
    - Private: only the object that owns the data can manipulate it
  - Methods of a class are defined by name, type of returned data, and types of all of the input data
  - GOOD practice: "namespace" entitites in your header files.

C++ example header

```
namespace ners570
{
  class timer {
    public:
        tic();
        toc();
    private:
      double startTime_;
      double totalTime_;
}
```

Usage

```
#include "ners570_timer.hpp"

//Declare variable "t" as a ners570
//timer, other headers might define
//classes named timer
ners590::timer t;
```

Execution Control Constructs

- IF/ELSE
  - Followed by curly braces { }, executes code within braces depending on result of conditional checks
  - `if (condition) { }`
- Switch
  - A logical branch, achieves the same logical result as IF/ELSE with much simpler syntax in some cases, and a different sequence of logical checks
    - `switch(variable):`
      - `case(value1)`
      - `case(value2)`
- `for(initialization, condition, step) {}`
  - Repeat code and execute step (usually increment/decrement) after each loop until the condition is no longer met

C and C++ I/O

C

- Routines are defined in "standard library", accessible through header files.
  - Primary library: `<stdio.h>`
- Some useful routines:
  - `printf`, `fprintf`
  - `fopen`, `fclose`, `fget`, `fscanf`

C++

- C++ I/O libraries: `<fstream>`, `<iostream>`
- `cout << "Hello, world!" << endl;`
  - Hello, world!
- `cout` outputs to screen, is in standard namespace (e.g. equivalent to `std::cout`, "`std::`" is implied)
- `cin <<` waits for input from the keyboard

Standard Library

- Different for C and C++
- ***A HUGE advantage over Fortran***
- Contains many useful types and functions
  - Example: `Vector`
    - a dynamic data container class with many methods for accessing more effectively than a standard array
    - `.push_back()`, `.pop_back()`, `.at()`, `.size()`
  - Dynamic memory management (`malloc`, `dmalloc`, `free`)
  - Random number generator (`rand`, `srand`, `RAND_MAX`)
  - `abs()` – absolute value
- Many other useful C libraries
  - `cstring`, `cmath`, `cstdio`

Angled brackets imply header is supplied by system or compiler

```
#include <vector>
#include "ners570_timer.hpp"
```

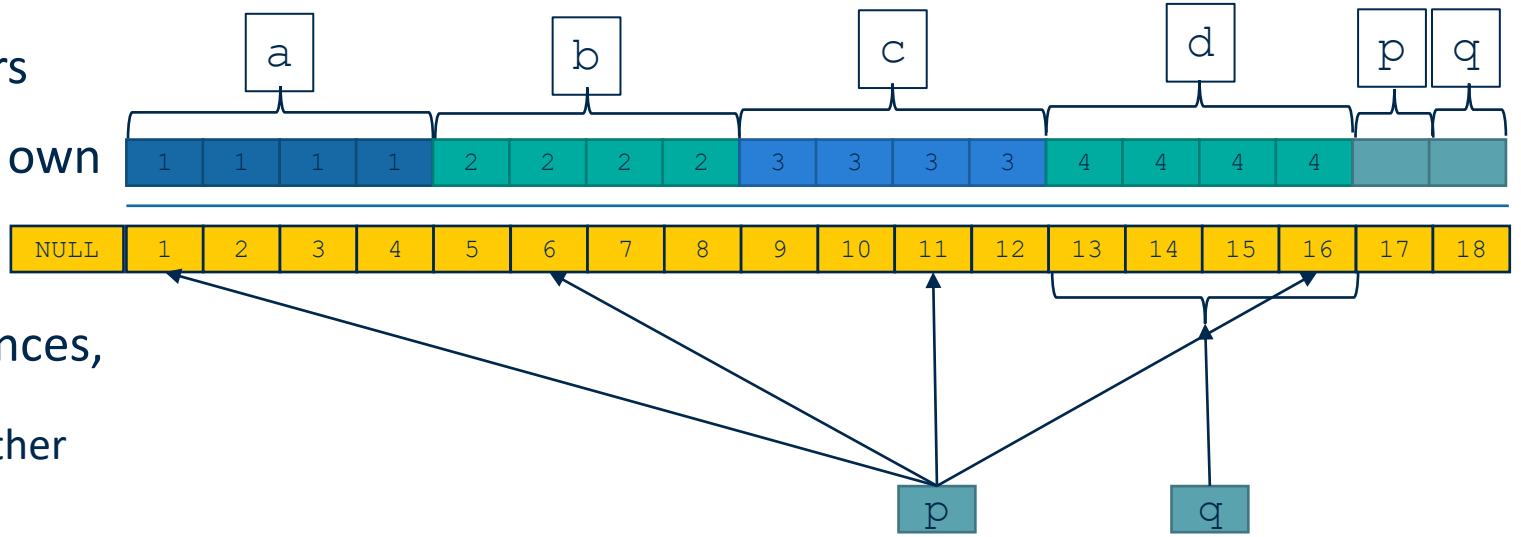
Quotes imply header file is source file defined by programmer

Pointers

- Difficult to grasp if new to programming.
- In high-level programming languages variable names are associated with memory.
  - value of variable is associated with memory location
- Variables that are defined as pointers can “point” to different memory locations and often don’t have their own associated memory.
- If a block of memory loses all references, this is a memory leak.
  - These are bad. More on these in another lecture.

```
integer a[4], b[4], c[4], d[4]
pointer p, q[]

p => a(1)
p => b(2)
p => c(3)
p => d(4)
q => d(:)
```



Reference Counted Pointers (RCP)

- Also known as a smart pointer.
  - Automates “garbage cleanup” e.g. frees unused memory
- Keeps track of (e.g. counts) how many pointers are referencing a particular block of memory
  - When no more pointers are referencing the block of memory, it can be automatically freed.
  - Useful machinery for helping to prevent memory leaks in C++

- Part of C++11 Standard: `std::shared_ptr`
- Other implementations available from third party libraries: boost, Trilinos

Templating (C++)

- ***Very powerful*** feature in C++
  - Idea is like meta-programming.
- Write a program for a "template" type.
- Compiler generates machine code for all data types matching the template.

```
class calc
{
  public:
    int multiply(int x, int y);
    int add(int x, int y);
};
int calc::multiply(int x, int y) { return x*y; }
int calc::add(int x, int y) { return x+y; }
```

```
template <class A_t> class calc
{
  public:
    A_t multiply(A_t x, A_t y);
    A_t add(A_t x, A_t y);
};

template <class A_t> A_Type calc<A_t>::multiply(A_t x,A_t y)
{
  return x*y;
}

template <class A_t> A_t calc<A_t>::add(A_t x, A_t y)
{
  return x+y;
}
```

Creating a Template means you have written this routine once for integers, floats, doubles, bools, and any classes of the templated type!

Example from: http://www.cprogramming.com/tutorial/templates.html

Further Reading

C

- The Language
- Standard Library

C++

- The Language
- Standard Library

Working with Fortran and C/C++ together

Interoperable Intrinsic Datatypes (Fortran 2003 and later)

Description	Fortran type declaration	C type declaration
Character	`CHARACTER(LEN=1,KIND=C_CHAR)`	`char`
True/False	`LOGICAL(C_BOOL)`	`_Bool`
default integer	`INTEGER(C_INT)`	`int`
floating point (32-bit)	`REAL(C_FLOAT)`	`float`
double precision (64-bit)	`REAL(C_DOUBLE)`	`double`
Integer 8-bit	`INTEGER(C_INT8_T)`	`int8_t`
Integer 16-bit	`INTEGER(C_INT16_T)`	`int16_t`
Integer 32-bit	`INTEGER(C_INT32_T)`	`int32_t`
Integer 64-bit	`INTEGER(C_INT64_T)`	`int64_t`
Long integer	`INTEGER(C_LONG)`	`long int`
Long long integer	`INTEGER(C_LONG)`	`long long int`

See documentation for ISO_C_BINDING module for complete listing.

Modules and Headers

- Fortran modules are like compiler generated header files
  - Makes Fortran a little bit more tricky to compile because modules must be compiled in the correct order to resolve dependencies.
  - Makes C/C++ a little more cumbersome because you are always having to maintain header files and source files.
- Header files are portable.
- *Compiled* module files are not.
- Fortran can also include "header files", but the `INCLUDE` keyword in Fortran implies a direct insertion (e.g. copy-paste) of the contents of an `INCLUDE` file.
  - Contents must be valid Fortran code
  - Typically used for defining types or global variables, sort of deprecated as a bad programming practice.

```
program main
  use module1
  use module2

  include 'file1.h'

  !Rest of program

end program
```

Modules "module1" and "module2" must have been compiled prior to compiling the program.

Other Things to keep in mind

Item	Fortran	C	C++
Case Sensitive variable names	No	Yes	Yes
Statements end with “;”	Optional	Required	Required
Assumed Starting Index	1	0	0
Multi-dimensional array ordering in memory	In-out	Out-in	Out-in
Strings	Fixed length	End with null character	

Memory layout of multi-dimensional arrays

Fortran

i ⟶

j ↓

a(i,j)	1	2
1	1	**2**
2	**3**	4

C/C++

i ⟶

j ↓

a[i][j]	0	1
0	1	**3**
1	**2**	4

Other things you'll encounter

Programming Language Extensions

- Includes things like
  - Syntax or Semantics not defined in the standard
    - An example is Co-array Fortran
      - Until Fortran 2008 standard
  - Additional functions
    - Interfaces to OS
- BEWARE
  - Extensions are usually not portable between compilers

Directives and Preprocessor

- Primarily applicable to high level languages with compilers
- Preprocessor
  - Happens before compilation
  - Can control what source code is compiled
  - Mechanism for portability
- Directives
  - can appear as comments or preprocessor commands
  - Allows for safe compilation when feature is not available.

Upcoming Assignments

Lab 2 – Bash and Python Scripting

- Searching (on your own outside of lab)
  - Use of grep and find
- Parametric Study (work through half of this in lab)
  - Steam Table Evaluation
  - Write same script in Bash and Python

Homework 1

- Write a LaTeX document
  - Suggest you use www.overleaf.com
- Develop the same program in C/C++ and Fortran
  - Index mapping and numbering with a space filling curve
- C/C++/Fortran Interoperability
  - Take previous program and call Fortran from C and C from Fortran