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COMPILING, BUILDING, AND INSTALLING PROGRAMS ON THE CLUSTER

Building Computer Programs

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- The process of converting a *human-readable* file to a *machine-readable* file.

C program (simple text file written in C programming language)

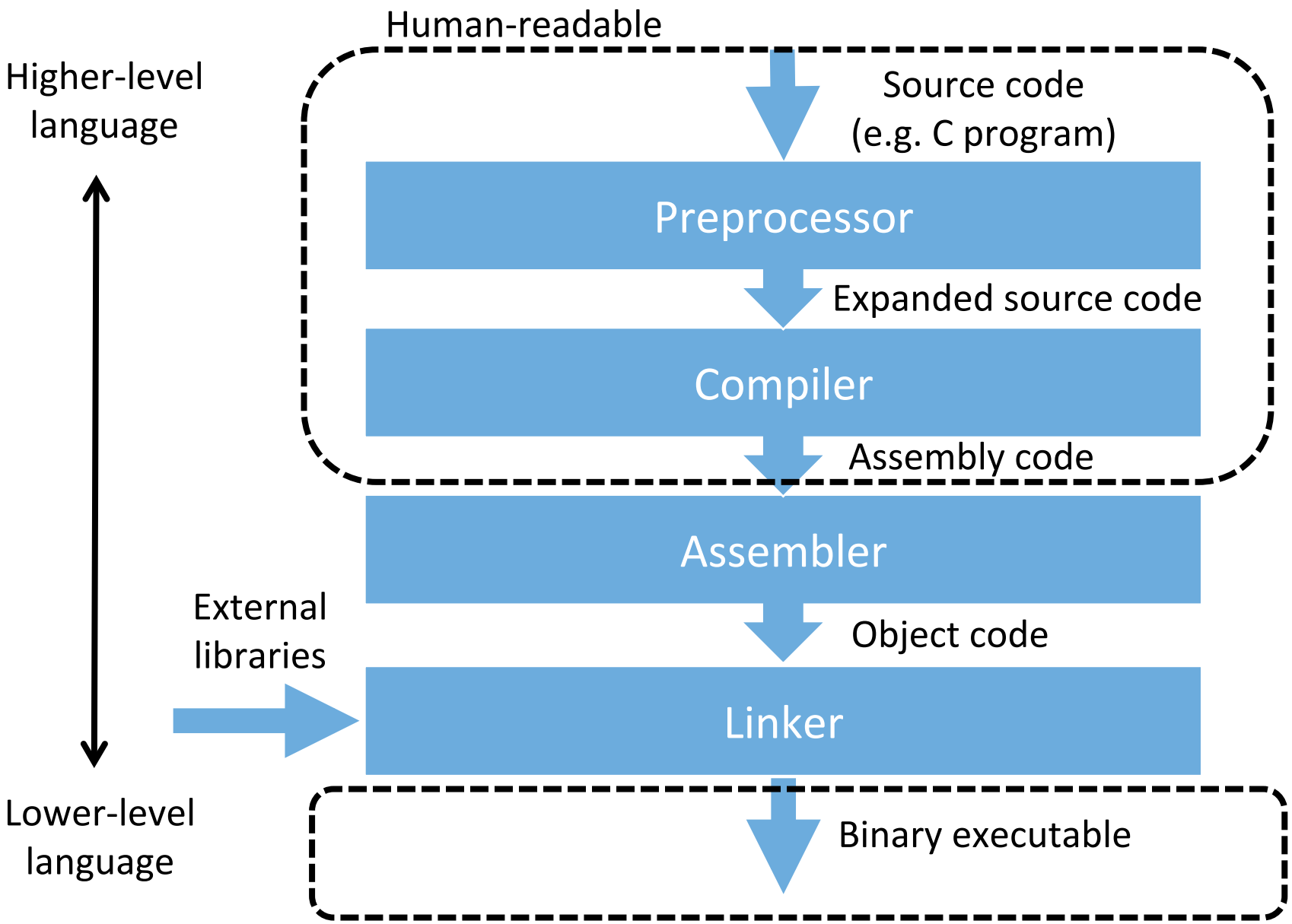
```
#include <stdio.h>

int main()
{
   printf("Hello World!\n");
   return 0;
}
```

Binary executable file (a set of CPU instructions encoded in 0's and 1's)

```
01010101000010101010 01
01011101010100101000 00
01011101010010110001 11
01101010101010101010
10100010101010101111 11
00101111011100001110 10
10101001111010101111 01
01010100001101010101 01
```

Sophisticated programs (e.g. a *compiler*) are used to perform this multi-step conversion.

The Build Process



Not all languages are compiled languages! The process to the left applies to programs written in C, C++, and Fortran.

PREPROCESSOR

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- Expands or removes special lines of code prior to compilation.

In C, preprocessor directives begin with the # symbol and are NOT considered C code.

Include statements:

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

- Copies contents of stdio.h into file.

Define statements:

```
.
.
#define PI 3.1415
.
.
```

- Replaces all instances of PI within file with 3.1415.

Header guards:

```
.
.
#ifndef FOO_H
#define FOO_H
#include “myHeader.h”
void myFunc(int);
#endif
.
.
```

- Prevents expanding multiple copies of the same header file by defining a unique “macro” for each header file.

Compiler

- Converts expanded source code to assembly code.

```
#include <stdio.h>

int main()
{
    printf("Hello World!\n");
    return 0;
}
```



```
.
.
main:
    .cfi_startproc
    pushq   %rbp
    .cfi_def_cfa_offset   16
    movq  %rsp  %rbp
.
.
```

Portability is an issue with compiled languages since assembly language contains instructions that are specific to a CPU's architecture.

- Assembly-level instructions are specific to a processor's Instruction Set Architecture (ISA).

- Example ISAs are x86, x86_64, and ARM. Most machines in HPC today support x86_64.

Assembler and Linker

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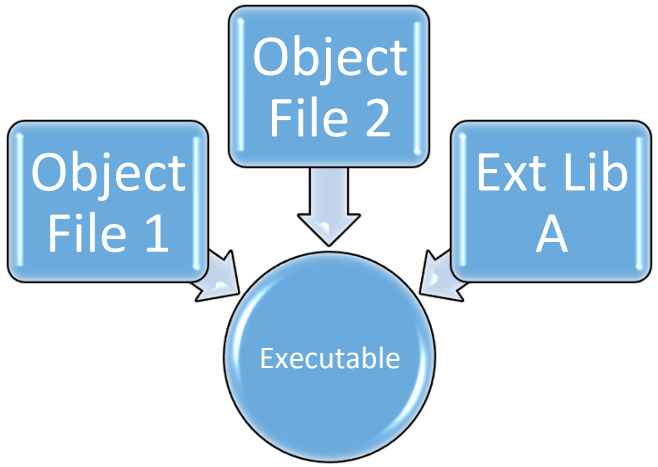
- **Assembler**: converts assembly code to object code.

  - Object code is in a binary format but cannot be executed by a computer's OS.
  - External libraries are often distributed as shared object files that are object code.
    - Hides specific implementation since these files are not human readable.
    - No need to be recompiled for each application that uses the library.
    - Stored efficiently in binary format.

- **Linker**: stiches together all object files (including any external libraries) into the final binary executable file.

  - Many applications often contain multiple source files, each of which need to be included in the final executable binary.
  - The job of the linker is to combine all these object files together into a final executable binary (a.k.a. "executable" or "binary") that can be run.



Using Compilers on the Cluster (1/3)

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IMPORTANT NOTE: In practice, the steps performed by the preprocessor, compiler, assembler, and linker are generally obscured from the user into a single step using (in Linux) a single command. In the next several slides, we will refer to this single command as a compiler, but note that we're actually talking about a tool that is a preprocessor + compiler + assembler + linker.

- **GCC: GNU Compiler Collection**
  - Free and open source
  - Most widely used set of compilers in Linux
  - C compiler: gcc
  - C++ compiler: g++
  - Fortran compiler: gfortran

```
$ pkginfo | grep gcc_compiler
                    gcc_compiler   GCC Compiler (4.6.1)
              gcc_compiler_4.9.0   GCC Compiler (4.9.0)
              gcc_compiler_4.9.3   GCC Compiler (4.9.3)
              gcc_compiler_5.2.0   GCC Compiler (5.2.0)
$ setpkgs -a gcc_compiler_5.2.0
$ gcc --version
gcc (GCC) 5.2.0
```

- **Intel Compiler Suite**
  - Licensed and closed source, but ACCRE purchases a license
  - Often produces faster binaries than GCC
  - Occasionally more difficult to build code due to lack of community testing
  - C compiler: icc
  - C++ compiler: icpc
  - Fortran compiler: ifort

```
$ pkginfo | grep intel_cluster_studio_compiler
 intel_cluster_studio_compiler   Intel Cluster Studio Co
mpiler (Including Intel MPI)
$ setpkgs -a intel_cluster_studio_compiler
$ icc --version
icc (ICC) 14.0.2 20140120
```

Using Compilers on the Cluster (2/3)

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```
gcc hello.c
```

- Builds C program with the GCC C compiler.
- Produces a binary called *a.out* that can be run by typing *./a.out*

```
gcc -o hello hello.c
```

- Produces a binary called *hello* that can be run by typing *./hello*

Error messages result when the build process fails. The compiler should provide details about why the build failed.

```
$ gcc -o hello hello.c
hello.c: In function ‘main’:
hello.c:33:4: error: expected ‘;’ before ‘return’
    return 0;
    ^
```

Warning messages occur when a program’s syntax is not 100% clear to the compiler, but it makes an assumption and continues the build process.

```
$ gcc -o hello hello.c
hello.c: In function ‘main’:
hello.c:23:4: warning: implicit declaration of function
‘printf’ [-Wimplicit-function-declaration]
    printf("Hello world!\n");
    ^
hello.c:23:4: warning: incompatible implicit declaration
 of built-in function ‘printf’
hello.c:23:4: note: include ‘<stdio.h>’ or provide a dec
laration of ‘printf’
```

Using Compilers on the Cluster (3/3)

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```
gcc -o hello -Wall hello.c
```

- *-Wall* will show all warning messages

```
gcc -E hello.c
```

- Show expanded source code

```
gcc -o hello -g hello.c
```

- *-g* will build the binary with debug symbols

```
gcc -S hello.c
```

- Create assembly file called *hello.s*

```
gcc -o hello -O3 hello.c
```

- *-O3* will build the binary with level 3 optimizations
- Levels 0 to 3 (most aggressive) available
- Can lead to faster execution times
- Default is −O0 in GCC and −O2 in Intel suite

```
gcc -c hello.c
```

- Create object file called *hello.o*

Vectorized loop execution is enabled with −O3 for GCC and −O2 for Intel.

```
icc -o hello -xHost hello.c
```

- Use Intel's C compiler to aggressively optimize for the specific CPU microarchitecture

Using the −xHost option leads to poor binary portability. Only use this option if you are sure the binary will always be executed on a specific processor type.

External Libraries (1/2)

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- **Statically Linked Library**: naming convention: liblibraryname.a (e.g. libcurl.a is a static curl library)

  - Linker copies all library routines into the final executable.
  - Requires more memory and disk space than dynamic linking.
  - More portable because the library does not need to be available at runtime.

- **Dynamically Linked Library**: naming convention: liblibraryname.so (e.g. libcurl.so is a dynamic curl library)

  - Only the *name* of the library copied into the final executable, not any actual code.
  - At runtime, the executable searches the LD_LIBRARY_PATH and standard path for the library.
  - Requires less memory and disk space; multiple binaries can share the same dynamically linked library at once.
  - By default, a linker looks for a dynamic library rather than a static one.

- **Do NOT need to specify the location of a library at build time if it's in a standard location (/lib64, /usr/lib64, /lib, /usr/lib). For example, libc.so lives in /lib64.**

External Libraries (2/2)

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- **Linking to libraries in non-standard locations requires the following information at build-time:**

  - Name of library (specified with −llibraryname flag)
  - Location of library (specified with −L/path/to/non/standard/location/lib)
  - Location of header files (specified with −I/path/to/non/standard/location/include)

```
gcc -L/usr/local/gsl/latest/x86_64/gcc46/nonet/lib -I/usr/local/gsl/latest/x86_64/
gcc46/nonet/include -lgsl -lgslcblas bessel.c -Wall -O3 -o calc_bessel
```

  - In this example, two libraries (gsl and gslcblas) are linked to the final executable.
  - Alternatively, use LIBRARY_PATH and C_INCLUDE_PATH to specify locations of libraries and headers.

- **Check the LD_LIBRARY_PATH and output of the *ldd* command before running the program:**

  - LD_LIBRARY_PATH shows list of directories that linker searches for dynamically linked libraries
  - Run *ldd ./my_prog* to see the dynamically linked libraries needed by an executable and the current path to each library

PORTABILITY

Can I build an executable on computer A and run it on computer B?

It depends! Are the platforms the same?

- CPU instruction set architecture (e.g. x86_64)
- Operating system
- External libraries

Platform

Support for specific vectorization extensions is also required for portability. For example, you cannot build a program with AVX2 on platform A and run it on platform B if AVX2 is not supported by platform B!

- This is why you often see different installers for different operating systems – the installer is simply copying a pre-built binary to your machine!
- Different CPU architectures are present on the cluster, so be sure to compile without overly aggressive optimizations or specify the target CPU architecture/family in your SLURM script
  (e.g. **#SBATCH --constrain=haswell**)

Other Compiler Fun Facts

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- **Many different compilers exist but not all compilers are created equal!**

  - GCC, Intel, Absoft, Portland Group (PGI), Microsoft Visual Studio (MSVS), to name a few.
  - Some are free, others are not!
  - It is not unusual (especially with large projects) for compiler A to build a program while compiler B fails.
  - Error messages and levels of verbosity can also vary widely.

- **Performance of program can be very compiler-dependent!**

  - This is especially true in scientific and high-performance computing involving a lot of numerical processing.
  - Compiler optimizations are especially tricky, sometimes the compiler needs help from the programmer (e.g. re-factoring code so the compiler can make easier/safer decisions about when to optimize code).
  - Some compilers (especially Intel's) tend to outperform their counterparts because they have more intimate/ nuanced information about a CPU's architecture (which are often Intel-based!).

Automating the Process: Makefiles (1/3)

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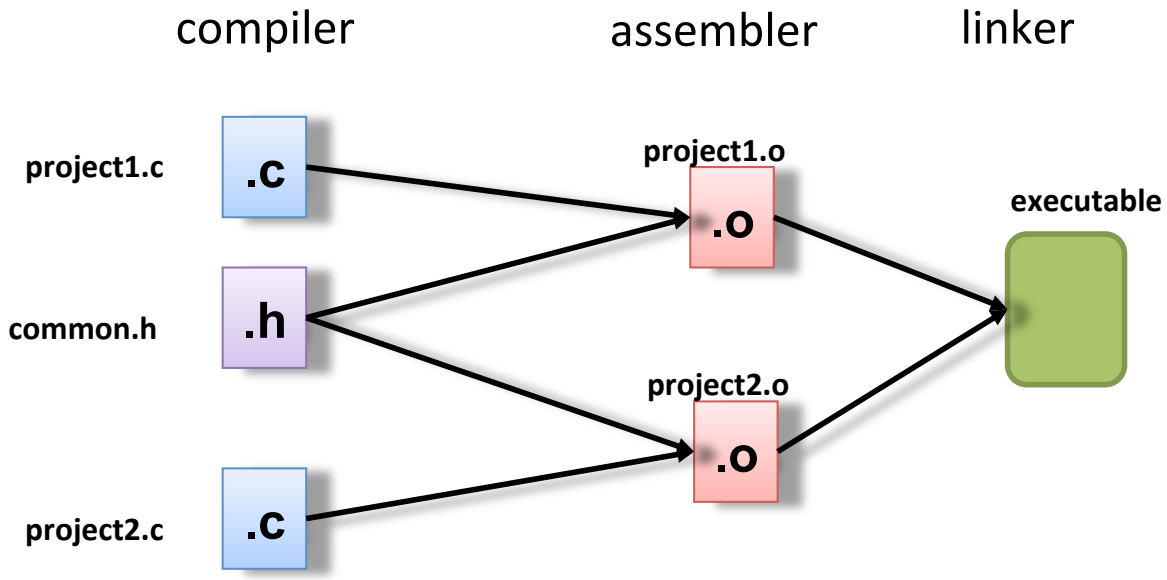
- **The Make tool allows a programmer to define the dependencies between sets of files in programming project, and sets of rules for how to (most often) build the project.**

- Default file is called Makefile or makefile.
- Allows build process to be broken up into discreet steps, if desired. For example, separate rules can be defined for (i) compiling+assembling, (ii) linking, (iii) testing, and (iv) installing code.
- Make analyzes the timestamps of a target and that target's dependencies to decide whether to execute a

By defining dependencies, you can avoid unnecessarily rebuilding certain files. For example, in the example on the right, project2.c does not need to be re-compiled if changes have been made to project1.c.



Automating the Process: Makefiles (2/3)

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- **Make analyzes the timestamp of a target's last modification and compares it to that of the target's dependencies to decide whether to execute the command(s) defined for that target's rule.**

Makefile Template

```
target: dependencies        # rule
<tab>    command1           # shell command
<tab>    command2           # shell command
.
.
```

- A "target" is a label/identifier for a rule
- Often the target is either the name of a file or a conventional rule (e.g. "install")
- Dependencies are files that the target depend on
- Commands must be preceded by a tab

Example Makefile (see previous slide)

```
executable: project1.o proect2.o
        gcc –o executable project1.o project2.o

project1.o: project1.c common.h
        gcc –c project1.c    # generates project1.o

project2.o: roject2.c common.h
        gcc –c project2.c    # generates project2.o
```

- There are often multiple rules defined per Makefile
- By just typing "make", the first rule in the file will be executed

Automating the Process: Makefiles (3/3)

```
$ ls
common.h  Makefile  project1.c  project2.c
$ make
gcc    -c -o project1.o project1.c
gcc    -c -o project2.o project2.c
gcc -o executable project1.o project2.o
$ make
make: `executable' is up to date.
$ touch project2.c
$ make
gcc    -c -o project2.o project2.c
gcc -o executable project1.o project2.o
$ make clean
rm -f project1.o project2.o executable
```

- Notice that Make is smart enough to not rebuild the program if no files have been modified since our last build.
- Make is also smart enough to only re-compile project2.c when it has been changed but project1.c has not.

To learn more about Makefiles, check out the following tutorial:
https://swcarpentry.github.io/make-novice/

`make`

- Generally builds the entire project.

`make clean`

- Deletes intermediate build files to start the build process from scratch.

`make test`

- Generally runs unit tests.

`make install`

- Generally installs the software.

"make install" generally fails with "permission denied" errors if you do not have administrative privileges or have not configured the build to install into a local directory.

Automating the Process: Configure Scripts (1/2)

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- **A configure script is an executable file responsible for building a Makefile for a project.**

- Determining the dependencies on a given system is difficult to predict and subject to constant change – writing a Makefile by hand for each system (or even a subset of representative systems) would be an enormous challenge and an administrative hassle.
- Instead, a configure script can be used to scan a system in search of all the needed dependencies (including versions of software, locations of external libraries), and build a Makefile that is specific to that system.
- Configure scripts are indispensible for large projects especially where the number of dependencies is large and difficult to manage/track.
- Alternatives to the configure script exist (cmake being the most common).

```
./configure
make
make test
make install
```

- Building projects on Linux at times this simple.
- Run only if you have administrative rights on system.

```
./configure --prefix=/my/local/dir
make
make test
make install
```

- --prefix option needed if installing in home directory on the cluster.

Automating the Process: Configure Scripts (2/2)

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- **Many configure scripts support a number of different options for configuring your build.**

```
./configure --help
```

- Show command line options.

```
$ ./configure --help
`configure' configures meep 1.2.1 to adapt to many kinds of systems.

Usage: ./configure [OPTION]... [VAR=VALUE]...

To assign environment variables (e.g., CC, CFLAGS...), specify them as
VAR=VALUE.  See below for descriptions of some of the useful variables.

Defaults for the options are specified in brackets.

Configuration:
  -h, --help              display this help and exit
      --help=short        display options specific to this package
      --help=recursive    display the short help of all the included packages
  -V, --version           display version information and exit
```

Make and Configure Macros

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- **There are a number of "macros" (think of as variables) that have standard meanings in Make and configure scripts. These macros can generally be exported as environment variables to customize your build.**

CC
- C compiler command (e.g. gcc)

CFLAGS
- C compiler flags (e.g. −Wall −O3)

CPP
- C preprocessor command (e.g. gcc)

CXX
- C++ compiler command (e.g. g++)

CXXFLAGS
- C++ compiler flags (e.g. −Wall −O3)

LDFLAGS
- Linker flags (e.g. −L/path/to/lib)

LIBS
- Library names (e.g. −lcurl)

FC
- Fortran compiler command (e.g. gfortran)

FFLAGS
- Fortran compiler flags (e.g. −O3)

MPICC
- MPI C compiler wrapper command (e.g. mpicc)

Compiled vs. Interpreted Languages

What about interpreted languages?

Compiled Language

- Faster execution time
- Slower development time
- Less portable
- C, C++, Fortran

Interpreted Language

- Slower execution time
- Faster development time
- More portable
- Python, Matlab, R, Ruby, Julia

The tradeoffs listed to the left are not universally true but in general apply.

Many popular modules/packages (e.g. NumPy, SciPy) loaded from interpreted languages are compiled shared object files and offer comparable performance to pure compiled languages.