

Lecture 04 – Elements of Development: *Configuring, Compiling, Linking*

Prof. Brendan Kochunas

NERS/ENGR 570 - Methods and Practice of Scientific Computing (F22)



COLLEGE OF ENGINEERING
NUCLEAR ENGINEERING & RADIOLOGICAL SCIENCES
UNIVERSITY OF MICHIGAN

Outline

- Motivation and Introduction
- Configuring
- Compiling
- Linking

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

- (*Knowledge*) explain what happens at each step of configuring, compiling, and linking
- (*Skill*) How to troubleshoot compilation
- (*Skill*) How to troubleshoot linking
- (*Knowledge*) explain dynamic vs static linking

Motivation

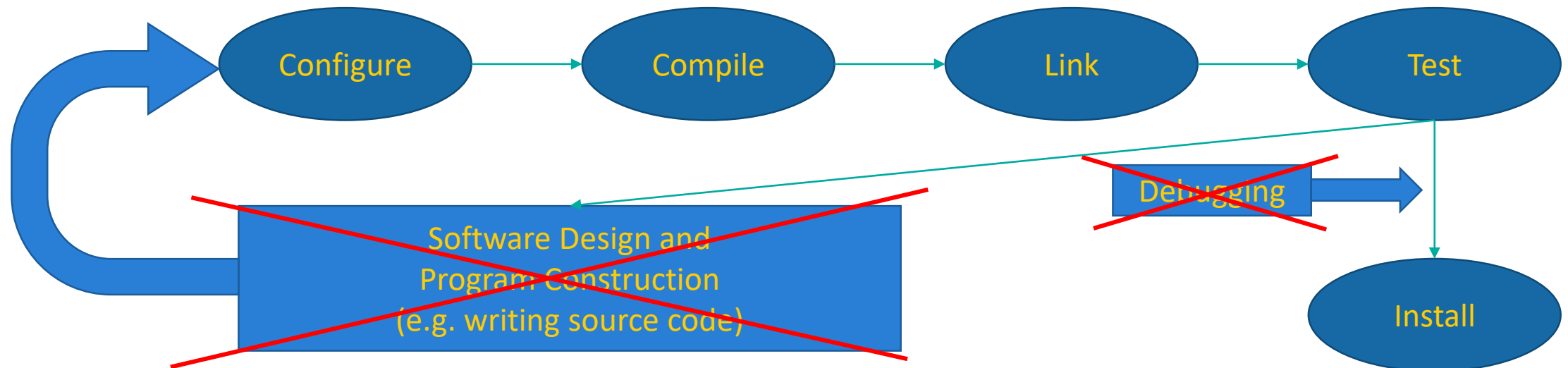
- How do we get other people to use our software?
- How do we use other people's software?
- We wish that it be as easy as:
 - apt-get install / yum install
 - conda install
 - python -m pip install --user
- Presently, this is not the case
 - HPCs are highly specialized machines
 - Some software is highly specialized



- This is a bigger problem that is being worked on

Elements to Development

- Program Design, Testing, and Debugging are all integral parts of development.
 - They each will get their own lecture later in the semester.
- This lecture is focused on the ***tools and steps*** needed to build software:



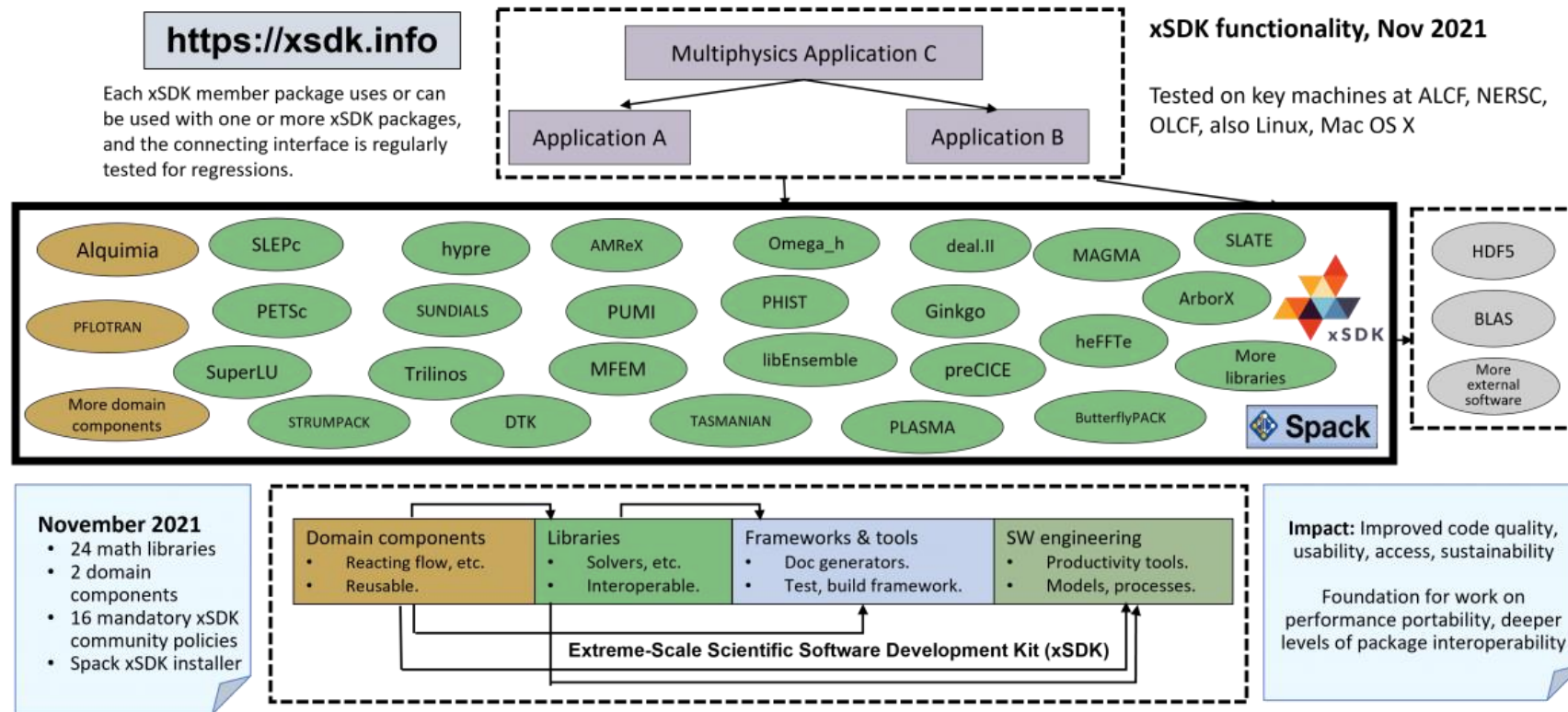
The “Toolchain”



- The tools (e.g. programs and their libraries) typically used by the developer that are needed to take your source files (as input) and produce executables.
- Frequently the definition of a tool chain will also include:
 - a program for “configuring”
 - a “make” script and compiler (compiler version and vendor matters)
 - a distribution of MPI
- Third Party Libraries (TPLs) are typically not considered part of the “toolchain”
 - MPI is sort of the exception to this
- Toolchains represent part of the “Minimum Requirements” for a software package.
 - Software packages can also support multiple toolchains

xSDK – Extreme-scale Scientific Software Development Kit

xSDK Version 0.7.0: November 2021



Some Terminology about “Time”

- *configure-time* – when you are configuring
 - *compile-time/build-time* – when you are compiling
 - *link-time* – when you are linking (very last step in “compiling”)
 - *run-time* – when you are running the executable
-
- Important for communicating “when things went wrong”

An Imperfect Cooking Analogy

Any volunteers that do not mind sharing details of their kitchen?



Configuring: Preparing to cook

Cooking

- Look around and find all the necessary ingredients and cookware (pots, pans, knives) to make dinner
 - Your stomach
 - Appliances
 - Spatula, spoon and knives
 - Salt, Pepper, Spices and Sauces
- Detailed instructions to cook in your kitchen
- Cookbooks
- Writing your own cookbook for others
- It's a part of life
- Use pre-packaged frozen meals

Software

- Purpose is to probe the system for to determine
 - the computer architecture (e.g. x86, AIX, ARM, etc.)
 - what compilers are installed, and where they are installed
 - what additional system software is installed
 - what third party libraries are available
- Basically creates “Makefiles” for a specific computer and environment for use in compiling (the next step)
- Specialized programs exist to perform the “configure” step.
 - autotools (autoconf/automake) → `configure`
 - CMake → `cmake`
- Most difficult part to establishing complex software systems.
- Considered part software infrastructure
- **AUTOMATE as much as possible**

Compiling: Cooking

Cooking

- Basically following the steps
 - Chop the onion
 - Season the
 - Fry the egg
 - Bake in the oven
- Lots of different kinds of steps/things we do in cooking
- Objective: prepare everything in the meal to go on the plate

Software

- Compilers do lots of different things.
 - Preprocessing
 - Optimizing
 - Check for errors
 - Give warnings
 - Generate assembly
 - Include this other file
- Objective: prepare all the machine code to go into the executable

Linking: Plating the Meal

Cooking

- Objective: put everything you've made together into a delicious meal.
- Considerations
 - Where did I put this cooked thing
 - Fresh parmesan?
 - Bowl or Plate
 - Spoon or Fork

Software

- Objective: put everything together into a functional executable
- Considerations
 - Where is this function/library coming from?
 - Library or executable
 - Shared or static



Configuring Software

Things that Configuring Can Control

- Where the libraries and executables produced from compilation are installed
- Compiler options:
 - e.g. whether the libraries and executables are “debug” (slow) or “release” (fast)
 - e.g. whether the compilation produces “dynamic” or “static” binaries
- What features of the library are enabled
 - e.g. with HDF5 you can specify whether you want the compiled library to include Fortran interfaces or just C interfaces.
 - e.g. what third party libraries to include (often provide additional capability in the software package)
 - In HDF5 the “Z” library can be included to provide data compression.
- Various other options that would be specific to the software package.

Configuration Options

The Cliff's Notes

- Depends on the tool!
- You will *always have to read documentation*
 - Usually files are named INSTALL or README
- Hopefully libraries and programs you work with are well documented
- Make sure you document your configuration steps well (or make them “robust”) in software you produce
 - People won't use your software if it is difficult to install or build.

“Common” Usage and Options

- Autotools (autoconf/automake)
 - `./configure [options]`
 - `--prefix=<path_to_install>`
 - `CC=<c_compiler>`
 - `FC=<fortran_compiler>`
- CMake
 - `cmake [options]`
`<path_source_dir>`
 - `-DCMAKE_BUILD_TYPE="Release"`
 - `-DCMAKE_C_COMPILER`
 - `-DCMAKE_CXX_COMPILER`
 - `-DCMAKE_Fortran_COMPILER`

Examples of Configuration Scripts

CMake (CMakeLists.txt) for METIS

```
cmake_minimum_required(VERSION 2.8)
project(METIS)

set(GKLIB_PATH "GKlib" CACHE PATH "path to GKlib")
set(SHARED FALSE CACHE BOOL "build a shared library")
if(MSVC)
    set(METIS_INSTALL FALSE)
else()
    set(METIS_INSTALL TRUE)
endif()
# Configure libmetis library.
if(SHARED)
    set(METIS_LIBRARY_TYPE SHARED)
else()
    set(METIS_LIBRARY_TYPE STATIC)
endif(SHARED)
include(${GKLIB_PATH}/GKlibSystem.cmake)
# Add include directories.
include_directories(${GKLIB_PATH})
# Recursively look for CMakeLists.txt in subdirs.
add_subdirectory("include")
add_subdirectory("libmetis")
add_subdirectory("programs")
```

Autoconf (configure.in) for PAPI

```
AC_PREREQ(2.59)
AC_INIT(PAPI, 5.5.0.0, ptools-perfapi@eecs.utk.edu)
AC_CONFIG_SRCDIR([papi.c])
AC_CONFIG_HEADER([config.h])

AC_MSG_CHECKING(for architecture)
AC_ARG_WITH(arch,
            [ --with-arch=<arch>   Specify architecture (uname -m)],
            [arch=$withval],
            [arch=`uname -m`])
AC_MSG_RESULT($arch)

AC_ARG_WITH(bitmode,
            [ --with-bitmode=<32,64> Specify bit mode of library],
            [bitmode=$withval])

AC_MSG_CHECKING(for OS)
```


Autotools Configure Example Cont.

```
#!/bin/sh
# Guess values for system-dependent variables and create Makefiles.
# Generated by GNU Autoconf 2.59 for PAPI 5.5.0.0.


# Identity of this package.
PACKAGE_NAME='PAPI'
PACKAGE_TARNAME='papi'
PACKAGE_VERSION='5.5.0.0'
PACKAGE_STRING='PAPI 5.5.0.0'
PACKAGE_BUGREPORT='ptools-perfapi@eecs.utk.edu'

ac_unique_file="papi.c"
# Factoring default headers for most tests.
ac_includes_default="\
#...
#if STDC_HEADERS
# include <stdlib.h>
# include <stddef.h>
#else
# if HAVE_STDLIB_H
# include <stdlib.h>
# endif
#endif
```

- As a user you typically will not **run** autoconf
 - But as a developer you might
- As a user you will run configure shell script produced by autoconf.
- Conventional wisdom for developers
 - CMake >> ~~Autoconf~~ Autotools
- **If starting new, start with CMake.**

Troubleshooting the Configure Step

For Scientific Software Development

- My configure failed! What do I do?
 - Uh oh... Usually difficult to resolve
- At best, problem is solved by modifying your environment.
- At worst, may require some other software be installed
 - And you may not have privileges to do so!
 - In this case you're likely 
 - ...unless you're willing to put in way more time than is appropriate

For Cooking

- I can't find everything I need to cook dinner!
 - I'm hungry now, but I need to grill this steak!
- Ask your neighbor for a cup of sugar and some eggs or a melon baller
- You mean I need a grill!?
 - But I live in an apartment!
 - Guess you'll go hungry
 - ...unless I can make friends with someone who has a grill



Configure Hands-on Example

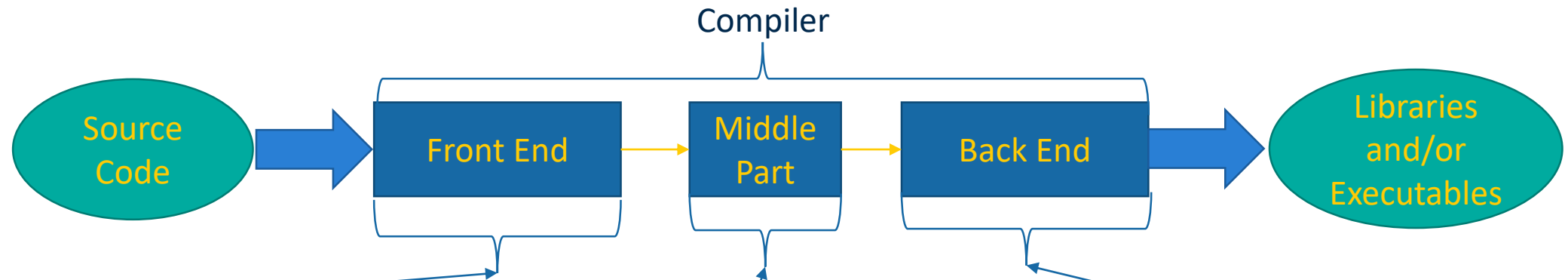


Compilers/Compiling

What is a Compiler?

- Translates a high-level programming language (suitable for humans) into a low level machine language required by the computer.
- Typically have several common features
 - Checking for syntax and programming errors
 - Supply debugging information
 - Perform optimizations
- It's a program written by people
 - so it has bugs
 - And different versions and the behavior between versions can vary significantly.

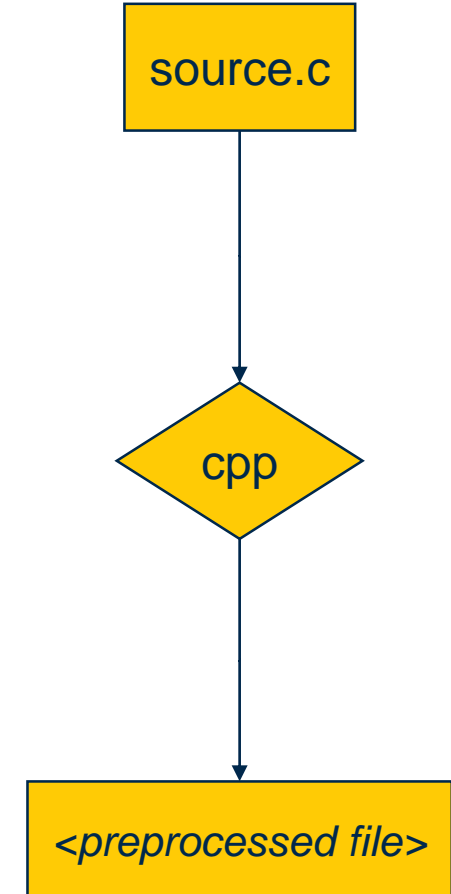
Modern Compiler Program Architectures



- Lexical Analysis
 - Read and parse text in source files into *tokens*
- Syntax Analysis
 - Arrange tokens in syntax tree to reflect program structure
- Type checking
 - Checks syntax tree for mistakes (e.g. undefined variables)
- Intermediate coded generation
 - Translation to simple machine independent language
 - Typically will vary between compilers
- Optimization
 - Apply algorithms for optimization to intermediate language
- Register allocation
 - Translate variables to machine registers (memory locations)
- Machine code generation
 - Translate intermediate language to machine code (assembly)
- Assembly and linking
 - Convert assembly to binary and resolve addresses for variables and functions

Other things a compiler does (sort of)

- Preprocess (separate program executed by compiler during compilation, “**cpp**”)
 - ***Modifies source files***
 - A part of C, but can be used in the compilation of C++ & Fortran
 - In Fortran file extensions control default behavior:
 - *.F, *.F90 are automatically preprocessed, and *.f, *.f90 are not
 - Based on “directives”, start with “#” in first column.
 - Include files, macro expansion, conditional compilation
 - Compilers will predefine some symbols for you
- Link (separate program executed by compiler during compilation, “**ld**”)
 - We’ll discuss linking in a few slides...



Some Preprocessor Examples

C

```
#include <stdio.h>

//Define macros
#define PI 3.14159
#define RADTODEG(x) ((x) * 57.29578)

int main()
{
    float x;
    x=RADTODEG(PI*0.5);
    printf("PI/2 radians in degrees is %.6f\n",x);
    return 0;
}
```

```
int main()
{
    float x;
    x=((3.14159*0.5) * 57.29578);
    printf("PI/2 radians in degrees is %.6f\n",x);
    return 0;
}
```

Fortran

```
PROGRAM main

#ifdef __GFORTRAN__
    WRITE(0,'(a,i2,a)') 'File: "'//__FILE__//'", line ',__LINE__, &
        " was compiled with gfortran!"
#else
    WRITE(0,'(a,i2,a)') 'File: "'//__FILE__//'", line ',__LINE__, &
        " was NOT compiled with gfortran!"
#endif

ENDPROGRAM
```

```
PROGRAM main

    WRITE(0,'(a,i2,a)') 'File: "'// "hello.F90"//'", line ',4, &
        " was compiled with gfortran!"

ENDPROGRAM
```


Compiler options for debugging

GCC compiler option	Meaning
<code>-g</code>	Produce debugging information in the operating system's native format (stabs, COFF, XCOFF, or DWARF). GDB can work with this debugging information.
<code>-fsanitize=<opt></code>	Enable AddressSanitizer, a fast memory error detector.
<code>-fbounds-check</code>	Generate additional code to check that indices used to access arrays are within the declared range during run time.
<code>-fcheck-pointer-bounds</code>	Each memory reference is instrumented with checks of the pointer used for memory access against bounds associated with that pointer.
<code>-fstack-check</code>	Generate code to verify that you do not go beyond the boundary of the stack.

Pretty much only `-g` is important.

For the other run-time checks, significant overhead in run time may be observed.

Other compiler options

GCC compiler option	Meaning
-C	Compile without linking
-o	Name of output file.
-I	Search path for included header files (there are predefined system paths)
-L	Search path for libraries
-l	Library name to link in
-D <i><symbol></i>	Define preprocessor symbol <i><symbol></i> during compilation
-E	Output preprocessed source file
-S	Output assembly from compilation
-fPIC	Compile P osition I ndependent C ode (necessary for shared objects)
-fopenmp	Process OpenMP directives
-p	Generate profiling information during run time for profiling analysis tools (e.g. <code>gprof</code>)
-ftest-coverage	Generate coverage information during run time for coverage analysis tools (e.g. <code>gcov</code>)

Object code & Binary output

- Compiling a source file `source.F90` (e.g. `-c`) produces an object file `source.o`
 - Object files are *relocatable* machine code.
 - Typical object file format for linux is ELF.
 - Cannot view object files in text editors
- ELF files contain
 - Program header table describing 0 or more segments
 - Contains run-time information
 - Section header table describing 0 or more sections
 - Contains link-time information
 - Data referred to by segments and sections
- How can you inspect ELF files/object code/object files?

Snippet of object file from
program on slide 15 in vi

[illegible]

Inspecting Object Files

readelf -a source.o

Symbol table '.symtab' contains 18 entries:

Num:	Value	Size	Type	Bind	Vis	Ndx	Name
0:	0000000000000000	0	NOTYPE	LOCAL	DEFAULT	UND	
1:	0000000000000000	0	FILE	LOCAL	DEFAULT	ABS	hello.F90
2:	0000000000000000	0	SECTION	LOCAL	DEFAULT	1	
3:	0000000000000000	0	SECTION	LOCAL	DEFAULT	3	
4:	0000000000000000	0	SECTION	LOCAL	DEFAULT	4	
5:	0000000000000000	0	SECTION	LOCAL	DEFAULT	5	
6:	0000000000000000	180	FUNC	LOCAL	DEFAULT	1	MAIN__
7:	0000000000000060	32	OBJECT	LOCAL	DEFAULT	5	options.1.1538
8:	0000000000000000	0	SECTION	LOCAL	DEFAULT	7	
9:	0000000000000000	0	SECTION	LOCAL	DEFAULT	8	
10:	0000000000000000	0	SECTION	LOCAL	DEFAULT	6	
11:	0000000000000000	0	NOTYPE	GLOBAL	DEFAULT	UND	_gfortran_st_write
12:	0000000000000000	0	NOTYPE	GLOBAL	DEFAULT	UND	_gfortran_transfer_charac
13:	0000000000000000	0	NOTYPE	GLOBAL	DEFAULT	UND	_gfortran_transfer_intege
14:	0000000000000000	0	NOTYPE	GLOBAL	DEFAULT	UND	_gfortran_st_write_done
15:	00000000000000b4	59	FUNC	GLOBAL	DEFAULT	1	main
16:	0000000000000000	0	NOTYPE	GLOBAL	DEFAULT	UND	_gfortran_set_args
17:	0000000000000000	0	NOTYPE	GLOBAL	DEFAULT	UND	_gfortran_set_options

nm source.o

```
0000000000000000 t MAIN__
                  U _gfortran_set_args
                  U _gfortran_set_options
                  U _gfortran_st_write
                  U _gfortran_st_write_done
                  U _gfortran_transfer_character_write
                  U _gfortran_transfer_integer_write
00000000000000b4 T main
0000000000000060 r options.1.1538
```

Wait... Why do I need to know what's in my object files?

97% of the time you don't need to know. However, this can be useful in resolving link errors and multi-language programs

Name Mangling (Fortran)

Fortran

- Binary symbol name is different from high level programming language name
- Variants:
 - Lower, Lower_, Lower__
 - Upper, Upper_, Upper__
- Used to be critical for calling Fortran from C.
 - Now the Fortran standard provides features that give programmer more control over name mangling.

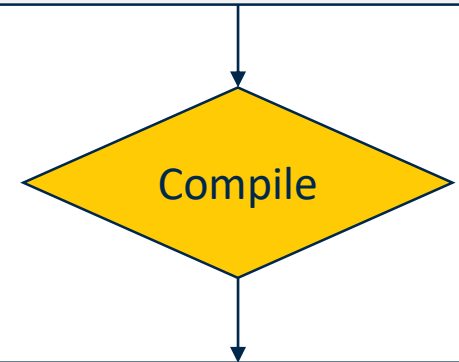
```
SUBROUTINE Sub1 (n) BIND (C, NAME="Sub1")  
...  
ENDSUBROUTINE
```



```
0000000000000000 T Sub1
```

Source File

```
SUBROUTINE Sub1 (n)  
...  
ENDSUBROUTINE
```



Object File

```
0000000000000000 T sub1_
```

This example is "Lower_"

Name Mangling (C++)

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

using namespace std;

template <typename T>
inline T const& Max (T const& a, T const& b)
{
    return a < b ? b:a;
}

int main ()
{
    int i = 39; int j = 20;
    cout << "Max(i, j): " << Max(i, j) << endl;

    double f1 = 13.5; double f2 = 20.7;
    cout << "Max(f1, f2): " << Max(f1, f2) << endl;

    string s1 = "Hello"; string s2 = "World";
    cout << "Max(s1, s2): " << Max(s1, s2) << endl;
    return 0;
}
```

- Shows up with templating
 - Have to produce different binary code for each templated type
 - Necessary for linking

```
000000000000001c6 t _Z41__static_initialization_and_destruction_0ii
U _ZNKs7compareERKSs
U _ZNSaIcEC1Ev
U _ZNSaIcED1Ev
U _ZNSolsEPFRSoS_E
U _ZNSolsEd
U _ZNSolsEi
U _ZNSsC1EPKcRKSaIcE
U _ZNSt8ios_base4InitC1Ev
U _ZNSt8ios_base4InitD1Ev
U _ZSt4cout
U _ZSt4endlIcSt11char_traitsIcEERSt13basic_ostreamIT_T0_ES6_
0000000000000000 b _ZStL8__ioinit
U _ZStlsISt11char_traitsIcEERSt13basic_ostreamIcT_ES5_PKc
0000000000000000 W _ZStltIcSt11char_traitsIcESaIcEEbRKSBtIT_T0_T1_ES8_
```

Example from: https://www.tutorialspoint.com/cplusplus/cpp_templates.htm



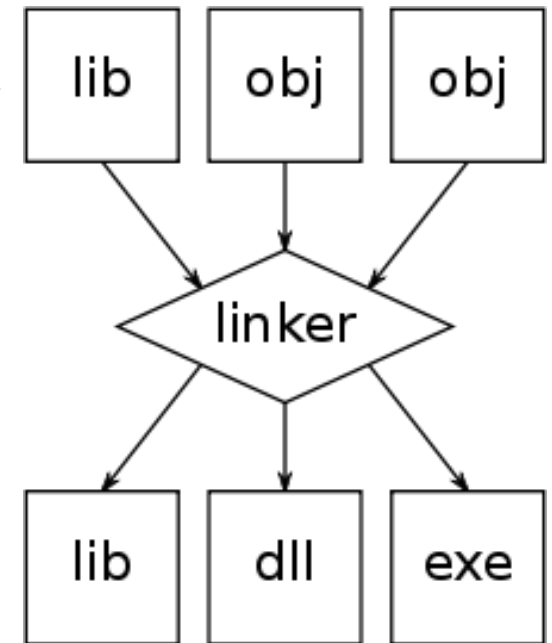
Compilation Hands-on Examples



Linking

What is Linking?

- Linking is the process of combining the various objects and libraries output from compilation into a single executable (or library or object).
 - May also include binaries (e.g. libraries) already installed on the system
- Sometimes performed by external program called by compiler (e.g. `ld`)
- Sometimes part of compiler (depends on the vendor)
- Key steps in linking are
 - *Resolving external symbols* that the linker uses to figure out how to piece together the executable
 - *Relocating load addresses* of various program parts (e.g. function addresses and variable addresses) to reflect the assigned addresses in the whole program.
- Linking can produce targets that are ***statically*** linked or ***dynamically*** linked



Dynamic Linking vs. Static Linking

Static Linking

- Probably what you think of when you think “linking”
- Copy all binary code from all libraries and objects then package into a single executable image
 - Usually results in larger executable file sizes
- A little more portable since all the binary code is packaged together
- Requires all libraries that are linked to be static libraries (e.g. `lib<name>.a`)
- Sometimes a requirement on large clusters
 - Compute nodes and login nodes are different

Dynamic Linking

- Symbol resolution is delayed until executable is run
 - Executable code has undefined symbols
 - Requires all libraries that are linked to be dynamic libraries (e.g. `lib<name>.so`)
- Some advantages
 - For system libraries used by every program, no need to copy into every executable (e.g. `libc`)
 - If there is a bug in a library, and a new version of the library that fixes the bug is installed, all programs benefit.
 - Statically linked executables need to be re-linked
- Some disadvantages
 - Libraries that are updated that break backwards compatibility, might break your executable.
 - Need to have the correct environment.
 - Not necessarily portable, OS and environment need to be consistent.

What link errors look like

Static Link Error

```
PROGRAM hello_main  
  
WRITE(*,*) "Hello World!"  
CALL some_undefined_routine()  
  
ENDPROGRAM
```

```
$ gfortran -c hello.F90  
$ gfortran hello.o -o hello.exe  
hello.o: In function `MAIN__':  
hello.F90:(.text+0x71): undefined reference to  
`some_undefined_routine_'  
collect2: ld returned 1 exit status
```

The command given to the linker did not include the library or object (or the correct path to the library or object) that defines the named symbol.

Dynamic Link Error

```
$ ./some_mpi_program.exe  
./mpi_program.exe: error while loading shared  
libraries: libmpi.so: cannot open shared object file:  
No such file or directory
```

When you attempted to run the executable,
The OS could not find the library using the
information in your current environment

How to trouble shoot link errors

Static Link Error

- Most likely you are missing the correct entries on the following options passed to the linker:
 - `-l<library_name_with_symbol>`
 - `-L<path_to_library>`
- Could also be a typo in your source code
- Generally easy to resolve
 - If you know where the missing library is located.
- Can be difficult if you have no idea why the symbol is trying to be linked (where is it used, where is it defined)
 - More likely to happen when you are linking third party libraries

Dynamic Link Error

- Most likely your environment is not the same as when you compiled
 - Check your environment
 - Environment variable is `LD_LIBRARY_PATH`
- Useful command: `ldd`
 - Shows you *exactly* what libraries are dynamically linked to your executable

```
$ ldd ./some_mpi_program.exe
linux-vdso.so.1 => (0x00007ffcf2be8000)
libmpi.so => not found
libc.so.6 => /lib/x86_64-linux-gnu/libc.so.6
(0x00007f4d12878000)
/lib64/ld-linux-x86-64.so.2 (0x00007f4d12c38000)
```

Dynamic Loading: Linking in code at run time

- Start your executable then load a library into memory.
 - Use case is “plugins”. An example might be linking proprietary correlations for material properties.
 - Can be done interactively. User could specify library name and function name as an input.
 - Challenging to list “available symbols” in library, although this can be done. But basically need to know what routine you want to call
- In Linux requires “dl” library.

```
#include <dlfcn.h>

void* sdl_library = dlopen("libSDL.so", RTLD_LAZY);
if (sdl_library == NULL) {
    // report error ...
} else {
    void* initializer = dlsym(sdl_library, "SDL_Init"); //extract library contents
    if (initializer == NULL) {
        // report error ...
    } else {
        // cast initializer to its proper type and use
        typedef void (*sdl_init_function_type)(void);
        sdl_init_function_type init_func = (sdl_init_function_type) initializer;
    }
}
```

https://en.wikipedia.org/wiki/Dynamic_loading

Multi-language Programs

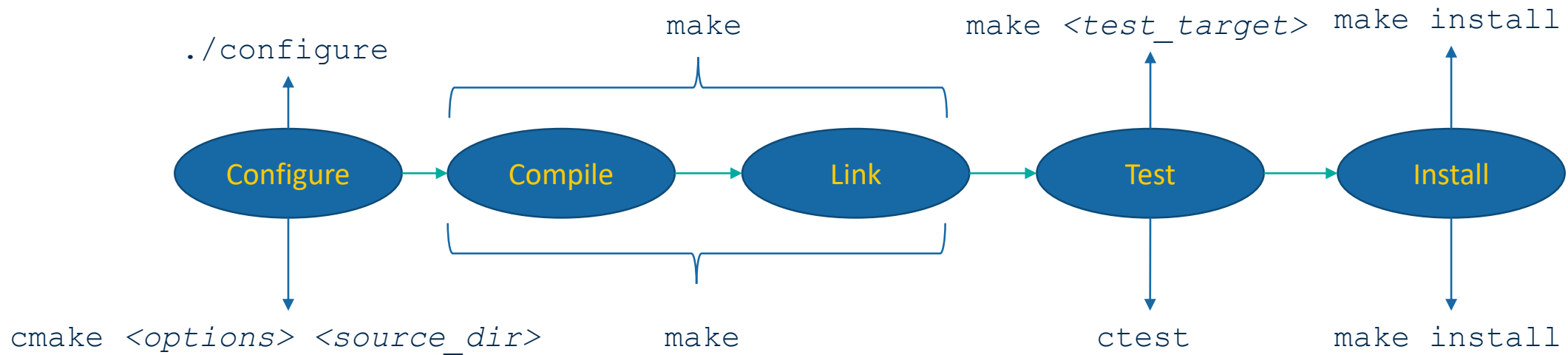
- **The key is linking!**
 - Linker does not care what high-level language produced your object code. It could have been generated from Fortran or C or C++.
 - Linker just has to resolve symbols in object code.
 - Well one subtlety, you must have a compatible application binary interface (ABI)
 - Usually not an issue unless you are compiling on one machine and linking on another.
- If a programming language or environment (e.g. Python) supports linking of C interfaces than you can link any code that provides a C interface
 - Most languages support C interfaces (because they were probably implemented in C or the compiler was)
 - Therefore, C is the de-factor language of interoperability.
- By “C interface” I mean a binary symbol that is producible from the C high-level language and a C compiler.



Linking Hands-on Example

Summary: Using the Toolchain

Autotools



CMake