Follow along with the examples...

```
[(it_nss:frey)@login00.darwin ~]$ mkdir ~/sw

[(it_nss:frey)@login00.darwin sw]$ git clone https://gitlab.com/jtfrey/unix-software-dev.git

[(it_nss:frey)@login00.darwin sw]$ git clone https://gitlab.com/jtfrey/unix-software-dev.git

[(it_nss:frey)@login00.darwin unix-software-dev]$ ls ~1

total 124

-rw-r-x-1 frey everyone 98 Sep 25 17:32 README.md

drvur-xx-x 2 frey everyone 15 Sep 25 17:32 src-1

drvur-xx-x 2 frey everyone 8 Sep 25 17:32 src-2

drvur-xx-x 2 frey everyone 8 Sep 25 17:32 src-3

drvur-xx-x 2 frey everyone 7 Sep 25 17:32 src-3

drvur-xx-x 4 frey everyone 7 Sep 25 17:32 src-5

drvur-xx-x 4 frey everyone 5 Sep 25 17:32 src-5

drvur-xx-x 4 frey everyone 5 Sep 25 17:32 src-5

drvur-xx-x 4 frey everyone 5 Sep 25 17:32 src-5

drwur-xx-x 4 frey everyone 5 Sep 25 17:32 valet-2.1
```

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HPC Software Development & Installation

HPC Software Development & Installation

Topics that will be covered:

- Software project kind & scope
- General organizational principles
- Compiled software projects
 - o Simple Makefile infrastructure
 - o GNU autoconf
 - o CMake

Additional topics, time permitting:

• Python virtual environments

- Varying degrees of scale to programming projects
 - o Tool programs
 - From a shell or Perl script to extract key data from an output file...
 - ...to a multi-file Fortran or Python program that post-processes (via computation) data from an output file

- Varying degrees of scale to programming projects
 - Tool programs
 - Code libraries
 - From a simple Unix archive file (e.g., libcompute.a) containing compiled object code...
 - ...to a dynamic shared library (e.g. libcompute.so) with a strong API exposed via header files.

- Many scripting (non-compiled) languages also have the concept of code libraries
 - Matlab .m files that add functions to the environment
 - Python modules (e.g. see /usr/lib64/python2.6/site-packages on Farber)
 - Perl modules (e.g. see /usr/lib64/perl5 on Farber)
- Note that creating an API demands more planning and structure to a project

- Varying degrees of scale to programming projects
 - Tool programs
 - Code libraries

 - header file

From a sim An application program interface (API) is a set of ...to a dynai routines, protocols, and tools for building software applications.

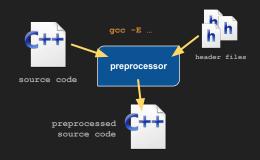
An API specifies how software components should

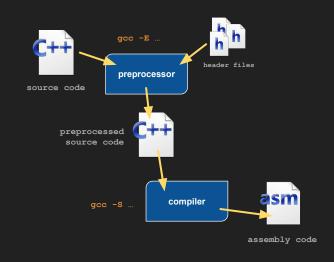
ı compiled object code... API exposed via

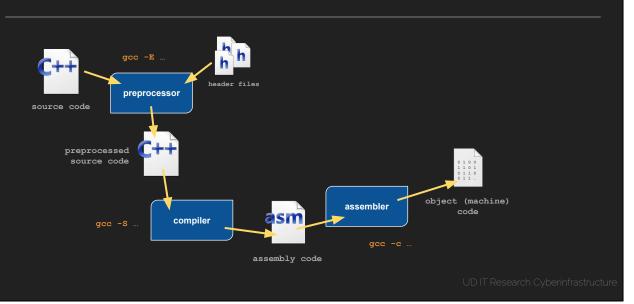
- Varying degrees of scale to programming projects
 - o Tool programs
 - Code libraries
 - Software suites
 - Containing a mix of tools and libraries

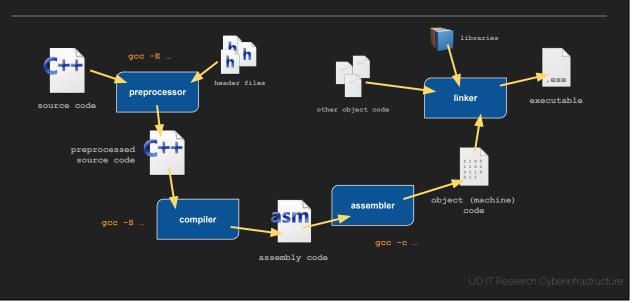
- Varying degrees of scale to programming projects
- A project that starts at the simpler end of the scale can evolve toward the complex end...
- ...or it could move between the types
 - o a collection of tool programs ⇒ library
 - a very complex tool program ⇒ software suite











- Note the gcc commands cited on the previous slide
 - o Output the preprocessed source and go no further...
 - o Output the assembly and go no further...

- Note the gcc commands cited on the previous slide
 - o Output the preprocessed source and go no further...
 - Output the assembly and go no further...
- Examine the preprocessed (.i) and assembly (.s) files
 - o Still textual program code
- Examine the object code with objdump -d exercise.o
- Examine the executable with readelf -a exercise
- Explore the other options available with these utilities (man pages)

```
[(it_nss:frey)@login00.darwin ~]$ gcc -E -o exercise.i exercise.c

[(it_nss:frey)@login00.darwin ~]$ gcc -S -o exercise.s exercise.i

[(it_nss:frey)@login00.darwin ~]$ gcc -c -o exercise.o exercise.s

[(it_nss:frey)@login00.darwin ~]$ gcc -o exercise exercise.o
```

- Any sufficiently advanced technology is indistinguishable from magic.
- Ex

Arthur C. Clarke's Third Law

- Examine the exercise
- Explore the other options available with these utilities (man pages)

```
[(it_nss:frey)@login00.darwin ~]$ gcc -E -o exercise.i exercise.c
[(it_nss:frey)@login00.darwin ~]$ gcc -S -o exercise.s exercise.i
[(it_nss:frey)@login00.darwin ~]$ gcc -c -o exercise.o exercise.s
[(it_nss:frey)@login00.darwin ~]$ gcc -o exercise exercise.o
```

- For a scientist, any technology that appears magical should prompt
- Ex curiosity and careful investigation.

Frey's Corollary to the Third Law

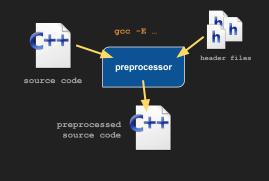
- Examine the constant with readelf -a exercise
- Explore the other options available with these utilities (man pages)

```
[(it_nss:frey)@login00.darwin ~]$ gcc -E -o exercise.i exercise.c

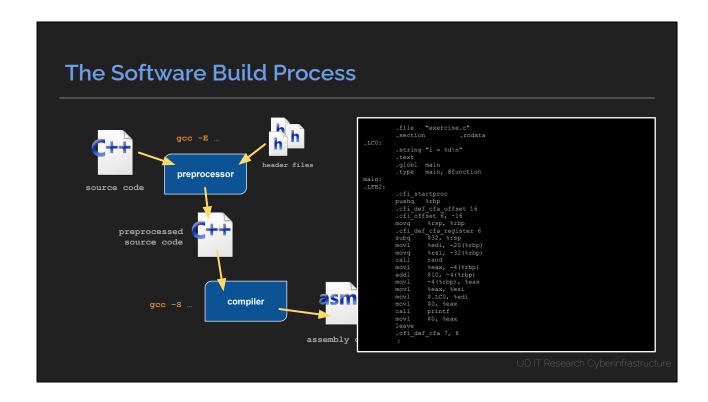
[(it_nss:frey)@login00.darwin ~]$ gcc -S -o exercise.s exercise.i

[(it_nss:frey)@login00.darwin ~]$ gcc -c -o exercise.o exercise.s

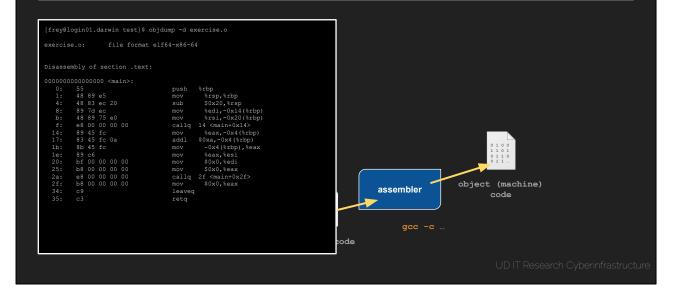
[(it_nss:frey)@login00.darwin ~]$ gcc -o exercise exercise.o
```



```
# 1 "exercise.c"
# 1 "<bullet-in>"
# 1 "<bullet-in>"
# 1 "<command-line>"
# 1 "/usr/include/stdc-predef.h" 1 3 4
# 1 "<command-line>" 2
# 1 "exercise.c"
# 1 "/usr/include/stdio.h" 1 3 4
# 1 "/usr/include/stdio.h" 3 4
# 1 "/usr/include/stdio.h" 3 4
# 1 "/usr/include/stdio.h" 3 4
# 1 "/usr/include/features.h" 3 4
# 1 "/usr/include/features.h" 3 4
# 1 "/usr/include/features.h" 1 3 4
# 375 "/usr/include/features.h" 1 3 4
# 3 932 "/usr/include/sys/cdefs.h" 3 4
# 1 "/usr/include/sys/cdefs.h" 3 4
# 1 "/usr/include/sys/cdefs.h" 3 4
# 1 "/usr/include/stdlib.h" 2 3 4
# 964 "/usr/include/stdlib.h" 3 4
# 3 "exercise.c" 2
int main(int argc, char* argv[])
{
    int i = rand();
    i = i + 10;
    printf("i = #d\n", i);
    return 0;
}
```



 Note that the code is now specific to the CPU on which you are building the software — the target ISA



General Organizational Principles

General Organizational Principles

- Any OS to which you've been exposed probably has the same solution to organizing files: a directory tree
 - o Top-most directory is most generic, sub-directory levels become increasingly specific

General Organizational Principles: Installed Software

- Top directory contains all *versions* or *variants* of the installed software
 - version: a frozen, point-in-time snapshot of software, often with a monotonically-increasing tiered numbering scheme (e.g. 4.5.1 or 2024.01)
 - o variant: a copy of a software version produced using alternative parameterization or build properties (e.g. 4.5.1 built with Intel versus GCC compilers)

General Organizational Principles: Installed Software

- Top directory contains all *versions* or *variants* of the installed software
- Each version or variant is a directory ideally structured similarly to the Linux file system
 - o bin directory to hold executable programs
 - o lib (or lib64) directory to hold archive or shared libraries, Python site packages, etc.
 - o include directory to hold header files (e.g. for an API)
 - o src if there is source code accompanying the version/variant
 - For software with multiple sources (e.g. library dependencies) unpack each source package under this directory
 - Notable exception is virtualized build systems (some autoconf, CMake)
 - Multiple versions/variants can be built in a single source directory outside the version/variant directory itself

General Organizational Principles: Source Code

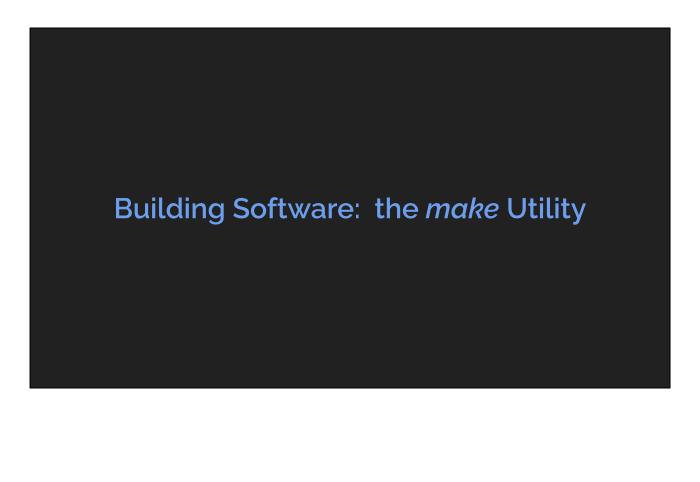
- Code is comprised of one or more files (be they source code or interpreted script, etc.)
- Top directory is the project container
 - Typical software project contains source code, documentation, helper scripts, configuration samples, examples
 - Create a directory for each that is required

General Organizational Principles: Source Code

- Code is comprised of one or more files (be they source code or interpreted script, etc.)
- Top directory is the project container

```
[(it_nss:frey)@login00.darwin ~]$ mkdir project
[(it_nss:frey)@login00.darwin ~]$ cd project
[(it_nss:frey)@login00.darwin project)$ mkdir src docs examples
[(it_nss:frey)@login00.darwin project)$ ls -1 .
total 11
dswxr-xr-x 2 frey everyone 2 Feb 23 12:40 docs
drwxr-xr-x 2 frey everyone 2 Feb 23 12:40 examples
drwxr-xr-x 2 frey everyone 2 Feb 23 12:40 src
```

- On our HPC systems we like to use "s-r-c" as the directory containing source
- code
 Content (or presence) of docs and examples will depend on each individual project



- Each source file depends on zero or more header/module files
 - When a dependency changes, the source file itself has effectively changed
 - my program depends directly on my program.c and printargv.c...
 - ...any change to printargv.c implies change to my program

```
[(it_nss:frey)@login00.darwin ~]$ cd ~/sw/unix-software-dev/src-1

[(it_nss:frey)@login00.darwin src-1]$ 1s -1

total 77

-tw-r--r- 1 frey everyone 115 Sep 25 17:32 Makefile.1

-tw-r--r- 1 frey everyone 274 Sep 25 17:32 Makefile.2

-tw-r--r- 1 frey everyone 274 Sep 25 17:32 Makefile.3

-tw-r--r- 1 frey everyone 274 Sep 25 17:32 Makefile.4

-tw-r--r- 1 frey everyone 280 Sep 25 17:32 Makefile.4

-tw-r--r- 1 frey everyone 280 Sep 25 17:32 Makefile.5

-tw-r--r- 1 frey everyone 180 Sep 25 17:32 Makefile.6

-tw-r--r- 1 frey everyone 193 Sep 25 17:32 makefile.6

-tw-r--r- 1 frey everyone 193 Sep 25 17:32 printargv.c

-tw-r--r- 1 frey everyone 198 Sep 25 17:32 printargv.h

-tw-r--r- 1 frey everyone 497 Sep 25 17:32 README.md
```

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 C, C++ languages provide API information via *header* files; Fortran 90 and later use *module* files for this purpose

- Each source file depends on zero or more header/module files
 - When a dependency changes, the source file itself has effectively changed
 - my program depends directly on my program.c and printargv.c...
 - ...any change to printargv.c implies change to my_program

```
[(it_nss:frey)@login00.darwin src-1]% cat Makefile.1

* Makefile for "my_program"

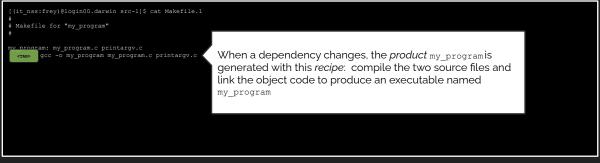
* my_program: my_program.c printargv.c

gcc -o my_program my_program.c printargv.c
```

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 A Makefile contains variable definitions and rules that combine product, ingredients, and a recipe to create the product from the ingredients.

- Each source file depends on zero or more header/module files
 - When a dependency changes, the source file itself has effectively changed
 - my program depends directly on my program.c and printargv.c...
 - ...any change to printargv.c implies change to my program



- Each source file depends on zero or more header/module files
 - o When a dependency changes, the source file itself has effectively changed
 - my program depends directly on my program.c and printargv.c...
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•

- Each source file depends on zero or more header/module files
 - When a dependency changes, the source file itself has effectively changed
 - my program depends directly on my program.c and printargv.c...
 - ...any change to printargv.c implies change to my program

```
[(it_nss:frey)@login00.darwin src-1]$ make -f Makefile.1
make: 'my_program' is up to date.

[(it_nss:frey)@login00.darwin src-1]$ touch printargv.c

[(it_nss:frey)@login00.darwin src-1]$ make -f Makefile.1
gcc -o my_program my_program.c printargv.c

[(it_nss:frey)@login00.darwin src-1]$ touch printargv.h

[(it_nss:frey)@login00.darwin src-1]$ make -f Makefile.1
make: 'my_program' is up to date.
```

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Why does "changing" printargv.h not trigger a rebuild of the program?

• The make utility is generally useful — not just for compiling code

```
[(it_nss:frey)@login00.darwin www]$ cat Makefile
manual.txt: man-sbatch.txt man-sacct.txt
    cat man-sbatch.txt man-sacct.txt > manual.txt

man-sbatch.txt:
    man -E ascii sbatch > man-sbatch.txt

man-sacct.txt:
    man -E ascii sacct > man-sacct.txt

[(it_nss:frey)@login00.darwin www]$ make
```

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 What happens when I execute the "make" command in this otherwise-empty directory?

• The make utility is generally useful — not just for compiling code

```
[(it_nss:frey)@login00.darwin www]$ cat Makefile
manual.txt: man-sbatch.txt man-sacct.txt
cat man-sbatch.txt man-sacct.txt
man-sbatch.txt:
man-E ascii sbatch > man-sbatch.txt
man-sacct.txt:
man-E ascii sacct > man-sacct.txt

[(it_nss:frey)@login00.darwin www]$ make
man-E ascii sacct > man-sbatch.txt
wan-E ascii sacct > man-sbatch.txt
cat man-sbatch.txt man-sacct.txt

[(it_nss:frey)@login00.darwin www]$ cat manual.txt
cat man-sbatch.txt man-sacct.txt > manual.txt
sbatch(1)

NAME

sbatch - Submit a batch script to Slurm.
;

First rule is the default rule for the Makefile

First rule is the default rule for the Makefile

With no -f <filename> the default Makefile/makefile is tried

Slurm Commands

sbatch(1)
```

• The make utility is generally useful — not just for compiling code

```
[(it_nss:frey)@login00.darwin www]$ rm manual.txt
[(it_nss:frey)@login00.darwin www]$ make
```

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Removing the manual.txt file — the default product — what will happen when I execute "make?"

• The make utility is generally useful — not just for compiling code

```
[(it_nss:frey)@login00.darwin www]$ rm manual.txt

[(it_nss:frey)@login00.darwin www]$ make
  cat man-sbatch.txt man-sacct.txt > manual.txt
```

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 No need to regenerate the two component .txt files, so the two files are concatenated to produce manual.txt

- The make utility is generally useful not just for compiling code
 - o Variables, automatic variables, and patterned rules simplify a Makefile

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- The make utility is generally useful not just for compiling code
 - o Variables, automatic variables, and patterned rules simplify a Makefile

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- The make utility is generally useful not just for compiling code
 - o Variables, automatic variables, and patterned rules simplify a Makefile

```
Automatic variables =

captured parts of the rule

man-s.txt:

s(man_cmd) s+ > se

[(it_nss:frey)@login00.darwin www]$ make
man = ascii sacct > man-sbatch.txt

s(man_cmd) s+ > se

[(it_nss:frey)@login00.darwin www]$ make
man = ascii sacct > man-sbatch.txt
man = bascii sacct > man-sacct.txt

cat man-sbatch.txt man-sacct.txt > manual.txt
```

- Improving rebuild workload
 - Retain compiler output object code as intermediates used in linking

```
[(it_nss:frey)@login00.darwin src-1] cat Makefile.2

# Makefile for "my_program"

my_program.o printargv.o

gcc -o my_program.o printargv.o

my_program.o: my_program.c printargv.h

gcc -c my_program.c

printargv.o: printargv.c printargv.h

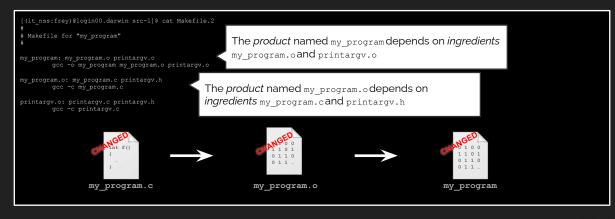
gcc -c printargv.c

printargv.o: printargv.c

my_program.o: my_program.o: my_program.o: my_program.o: depends on ingredients my_program.o: and printargv.h

my_program.o: my_program.o: depends on ingredients my_program.o: and printargv.h
```

- Improving rebuild workload
 - o Retain compiler output object code as intermediates used in linking



What gets rebuilt when printargv.h has changed?

- Improving rebuild workload
 - o Retain compiler output object code as intermediates used in linking

- Decrease repetition, increase readability
 - o Use *variables* for long or repeated values in the Makefile text

```
[frey@login00.darwin src-1]$ cat Makefile.3

# Makefile for "my_program"

# TARGET = my_program

OBJECTS = printargv.o my_program.o

$ (TARGET): $ (OBJECTS)

gcc -0 $ (TARGET) $ (OBJECTS)

my_program.o: my_program.c printargv.h

gcc -c my_program.c

printargv.o: printargv.c printargv.h

gcc -c printargv.c printargv.h
```

- Decrease repetition, increase readability
 - o Use *variables* for long or repeated values in the Makefile text

```
[frey@login00.darwin src-1] cat Makefile.3

# Makefile for "my_program"

# TARGET = my_program

OBJECTS = printargv.o my_progra

$(TARGET): $(OBJECTS)
gcc -0 $(TARGET) $(OBJECTS)
gcc -0 $(TARGET) $(OBJECTS)
my_program.o: my_program.c printargv.h
gcc -c my_program.c

printargv.o: printargv.c printargv.h
gcc -c printargv.c
```

- Decrease repetition, increase readability
 - Automatic variables yield components of the matched rule

- Decrease repetition, increase readability
 - o Automatic variables yield components of the matched rule

```
[frey@login00.darwin src-1] cat Makefile.4

# Makefile for "my_program"

TARGET = my_program

OBJECTS = prints
$(TARGET): $(OBJECTS)
gcc -0 $@ $+

my_program.o: my_program
gcc -0 $<

printargv.o: printars
gcc -0 $<

printargv.o: printars
gcc -0 $<
```

 Google for the term "makefile automatic variables" for more information on what's available

- Pattern-based rules
 - o Another means of avoiding repetition, increasing readability

```
[frey@login00.darwin src-1] cat Makefile.5

* Makefile for "my_program"

*

TARGET = my_program

OBJECTS = printargv.o my_program.o

$ (TARGET): $ (OBJECTS)
    gcc -o $0 $+ $ (LDELAGS) $ (LIBS)

my_program.o: my_program.c printargv.h

printargv.o: printargv.c printargv.h

*.o: *.c

    gcc -c $ (CFFFLAGS) $ (CFLAGS) $
```

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Automatic variables are absolutely necessary for pattern-based rules

- Pattern-based rules
 - o Another means of avoiding repetition, increasing readability

- Additional targets
 - o Rules that effect other changes to the build products et al.

- Additional targets
 - o Rules that effect other changes to the build products et al.

- Additional targets
 - o Rules that effect other changes to the build products et al.

- After all of that, what **does** this program actually do????
- We're now done with the basics of Makefiles

- Multi-tier source projects a library and an executable
 - o Encapsulate global definitions in separate files

```
[frey@login00.darwin src-2] cat Makefile.inc

# Makefile.inc
# Global variables for subprojects
#

MAKEFILE_INC :=$(abspath $(lastword $(MAKEFILE_LIST)))

SRCDIR :=$(dir $(MAKEFILE_INC))

CC = goc
CPPELAGS += -DVERSION=1.0

CFLAGS += -JUSSION=1.0

LDFLAGS += -Lusr/lib64

LIBS += -Im

[frey@login00.darwin src-2] cat Makefile.rules
#

Makefile.rules
# Templated rules used by subprojects
#

%.o: %.c
gcc -c $(CPPFLAGS) $(CFLAGS) $<
```

- Multi-tier source projects a library and an executable
 - o Encapsulate global definitions in separate files

```
[frey@login00.darwin src-2]% cat Makefile

# Top-level Makefile for subproject

# SUBPROJS = libprintargv my_program

default:

@for SUBPROJ in %(SUBPROJS); do make -c %%SUBPROJ; done

clean:

@for SUBPROJ in %(SUBPROJS); do make -c %%SUBPROJ clean; done
```

- Multi-tier source projects a library and an executable
 - The include command inserts another file's content at that location

- Multi-tier source projects a library and an executable
 - The include command inserts another file's content at that location

```
[frey@login00.darwin src-2]$ cat libprintargy/Makefile

# Makefile for 'libprintargy' subproject

# include ../Makefile.inc

TARGET = libprintargy.a

OBJECTS = printargy.o

default: $(TARGET)

clean:

$(RM) $(TARGET) $(OBJECTS)

$(ARG) cr $(TARGET) $(OBJECTS)

printargy.o: printargy.c printargy.h

include ../Makefile.rules

The ar utility creates/updates a static archive, a single file containing (in this case) the object intermediates
```

- A *static library* is just a special file containing a collection of object code files emitted by a compiler
- The code in the static library is added directly to any executable that links against it — in contrast to *shared libraries* which only add a reference to the executable
 - When using shared libraries, the library must be present BOTH at build and run time; a static library is not needed at run time

- Multi-tier source projects a library and an executable
 - The include command inserts another file's content at that location

- A static library is just a special file containing a collection of object code files emitted by a compiler
- The code in the static library is added directly to any executable that links against it — in contrast to *shared libraries* which only add a reference to the executable
 - When using shared libraries, the library must be present BOTH at build and run time; a static library is not needed at run time

- Exercise: let's add an install target to the build infrastructure
 - 1. Variables: use a variable named PREFIX for the base install path
 - Default to /usr/local
 - 2. Add an "install" target to Makefile that invokes make install in subdirectories
 - 3. Add an "install" target to subdirectories' Makefile
 - libprintargv
 - Copy header file to \$ (PREFIX) / include
 - Copy static library to \$ (PREFIX) / lib
 - my_program
 - Copy executable to \$ (PREFIX) /bin

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lacktriangle

 Variables: use a variable named PREFIX for the base install path

```
[frey@login00.darwin src-2]$ vi Makefile.inc

# Makefile.inc
# Global variables for subprojects
#

FREFIX ?= /usr/local

MAKEFILE_INC := % (abspath $ (lastword $ (MAKEFILE_LIST)))

SRCDIR := % (dir $ (MAKEFILE_INC))

CC = gcc

CPPFLAGS += -DVERSION=1.0

CFLAGS += -g -O3

LDFLAGS += -L/usr/lib64

LIBS += -lm
```

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- 1. Variables: use a variable named PREFIX for the base install path
- 2. Add an "install" target to Makefile that invokes make install in subdirectories

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- 1. Variables: use a variable named PREFIX for the base install path
- 2. Add an "install" target to Makefile that invokes make install in subdirectories
- Add an "install" target to subdirectories' Makefile
 - libprintargv

```
[frey@login00.darwin src-2]$ vi libprintargv/Makefile

# Makefile for 'libprintargv' subproject

# include ../Makefile.inc

TARGET = libprintargv.a

OBJECTS = printargv.o

default: $(TARGET)

clean:
    $(RM) $(TARGET) $(OBJECTS)

install: $(TARGET)
    cp printargv.h $(PREFIX)/include
        cp $(TARGET) $(PREFIX)/lib

#

$(TARGET): $(OBJECTS)
    $(AR) cr $(TARGET) $(OBJECTS)

printargv.o: printargv.c printargv.h

include ../Makefile.rules
```

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Building Software: the make Utility 1. Variables: use a variable named PREFIX for the base install path 2. Add an "install" target to Makefile that invokes make install in subdirectories This will fail because the destination directories do not necessarily exist! O LIDPTINEARGY INSURABLE : (TARGET) | (OBJECTS) | (OBJECTS) | (OBJECTS) | (TARGET) | (TARG

 Could just also include "mkdir" commands in the "install" recipe, but why not leverage make dependencies to ONLY do so when necessary?

- 1. Variables: use a variable named PREFIX for the base install path
- 2. Add an "install" target to Makefile that invokes make install in subdirectories
- Add an "install" target to subdirectories' Makefile
 - libprintargv

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- 1. Variables: use a variable named PREFIX for the base install path
- 2. Add an "install" target to Makefile that invokes make install in subdirectories
- 3. Add an "install" target to subdirectories' Makefile
 - libprintargv
 - o my_program

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• Give it a try!

```
[frey@login00.darwin src-2]$ make clean
make[1]: Entering directory '/home/1001/sw/unix-software-dev/src-2/libprintargv'
rm -f libprintargv.a printargv.
make[1]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/libprintargv'
make[1]: Entering directory '/home/1001/sw/unix-software-dev/src-2/my_program'
rm -f my_program my_program.o
make[1]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/my_program'

[frey@login00.darwin src-2]$ make
make[1]: Entering directory '/home/1001/sw/unix-software-dev/src-2/libprintargv'
gcc -c-DVERSION-1.0 -G -O3 printargv.c
ar or libprintargv.a printargv.c
ar cr libprintargv.a printargv.c
make[1]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/libprintargv'
make[1]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/my_program'
gcc -c-DVERSION-1.0 -1/home/1001/sw/unix-software-dev/src-2/my_program'
gcc -g -O3 -o my_program my_program.o -L/usr/lib64 -L/home/1001/sw/unix-software-dev/src-2/libprintargv -lm -lprintargv
make[1]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/my_program'
```

• Give it a try!

```
[frey@login00.darwin src-2]% make install
make[i]: Entering directory '/home/1001/sw/unix-software-dev/src-2/libprintargv'
op printargy.h /usr/local/include
op: cannot create regular file '/usr/local/include/printargv.h': Permission denied
make[i]: *** [install] Error 1
make[i]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/libprintargv'
make[i]: Entering directory '/home/1001/sw/unix-software-dev/src-2/my_program'
op my_program /usr/local/bin
op: cannot create regular file '/usr/local/bin/my_program': Permission denied
make[i]: *** [install] Error 1
make[i]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/my_program'
make: *** [install] Error 2
```

• Give it a try!

• What if we "change" a source file?

```
[frey@login00.darwin src-2]$ make PREFIX=/tmp/xyz install
make[1]: Entering directory '/home/1001/sw/unix-software-dev/src-2/libprintargv'
gcc -c-DVERSION=1.0 -g -03 printargv.c
ar cr libprintargv.a printargv.c
cr printargv.a printargv.o
cp printargv.a /tmp/xyz/include
cp libprintargv.a /tmp/xyz/lib
make[1]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/myprogram'
gcc -c-DVERSION=1.0 -I/home/1001/sw/unix-software-dev/src-2/libprintargv -g -03 -o my_program my_program.o -L/usr/lib64 -L/home/1001/sw/unix-software-dev/src-2//libprintargv -lm -lprintargv
cp my_program /tmp/xyz/sin
make[1]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/my_program'

scc -c-DVERSION=1.0 -I/home/1001/sw/unix-software-dev/src-2/my_program /tmp/xyz/sin
make[1]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/my_program'
```

- The "install" target doesn't just install, it rebuilds some of the underlying components — what causes "make" to do that??
 - Since the "install" targets depend on the products, when changes affect those products "make" triggers those actions first

• What if we "change" a source file?

```
[frey@login00.darwin src-2]$ touch libprintargv.c

[frey@login00.darwin src-2]$ make FREFIX=/tm
make[i]: Entering directory '/home/1001/sw/un
gc -e -DVERSION=1.0 = -3 printargv.c
ar cr libprintargv.a printargv.c
ar cr libprintargv.a /tmp/xyz/include
cp libprintargv.a /tmp/xyz/include
cp libprintargv.a /tmp/xyz/lib
make[i]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/inprintargv'
make[i]: Entering directory '/home/1001/sw/unix-software-dev/src-2/libprintargv - 3 my_program my_program my_program.o -L/usr/lib64 -L/home/1001/sw/unix-software-dev/src-2//libprintargv - lm -lprintargv
cp my_program /tmp/xyz/bin
make[i]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/my_program'

gcc - -DVERSION=1.0 - I/home/1001/sw/unix-software-dev/src-2/my_program.

gcc - g - 0-3 - o my_program my_program.o -L/usr/lib64 -L/home/1001/sw/unix-software-dev/src-2/my_program'
make[i]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/my_program'
```

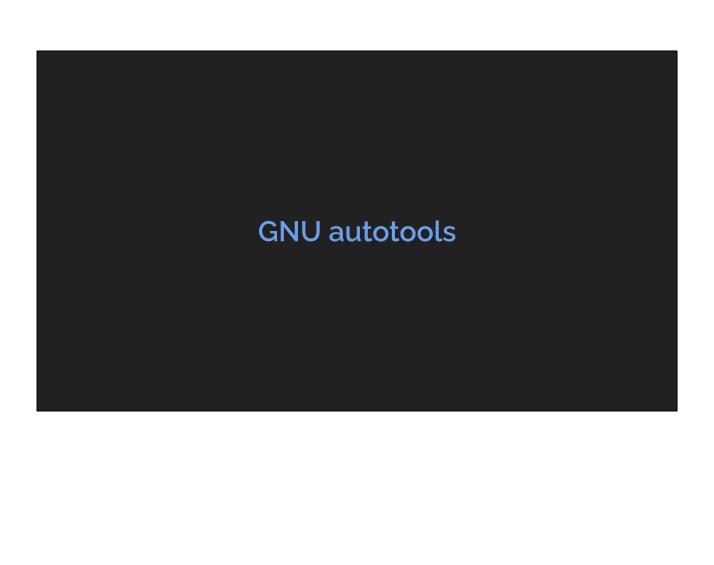
• What if we "change" a source file?

```
[frey@login00.darwin src-2]$ touch libprintargy/printargy.c

[frey@login00.darwin src-2]$ make PREFIX=/tmp/xyz install
make[1]: Entering directory '/home/1001/sw/unix=software-dev/src-2/libprintargy'
gcc -c-DVERSION=1.0 -g -03 printargy.c
ar cr libprintargy.a printargy.c
op printargy.a /tmp/xyz/include
cp libprintargy.a /tmp/xyz/lib
make[1]: Leaving directory '/home/1001/sw/unix-software-dev/src-2/libprintargy '
make[1]: Entering directory '/home/1001/sw/unix-software-dev/src-2/libprintargy -g -03 my_program my_program.c
gcc -c-DVERSION=1.0 -1/home/1001/sw/unix-software-dev/src-2//libprintargy -g -03 my_program my_program.c -1/usr/lib64 -1/home/1001/sw/unix-software-dev/src-2//libprintargy -lm -lprintargy
cp my_program /tmp/xyz/bin

The change to the static library causes my_program to be relinked — why
is this necessary?
```

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GNU autotools

- Writing and maintaining Makefiles by hand can become cumbersome
 - A lot of what we embedded in Makefile.inc and Makefile.rules is likely common to almost all projects
 - A lot of what we did by hand could be automated
 - For each source file, determine on what other files it depends (e.g. headers)
 - E.g. gcc ... -MMD ... to emit make-style dependency files

- Writing and maintaining Makefiles by hand can become cumbersome
 - A lot of what we embedded in Makefile.inc and Makefile.rules is likely common to almost all projects
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 - For each source file, determine on what other files it depends (e.g. headers)
 - E.g. gcc ... -MMD ... to emit make-style dependency files

```
[frey@login00.darwin src-2]$ make
: gcc -c -DVERSION=1.0 -MMD -g -03 printargv.c
: gcc -c -DVERSION=1.0 -MMD -I/home/1001/sw/unix-software-dev/src-2//libprintargv -g -03 my_program.c
:
[frey@login00.darwin src-2]$ cat libprintargv/printargv.d
printargv.o: printargv.c printargv.h

[frey@login00.darwin src-2]$ cat my_program/my_program.d
my_program.c: my_program.c \\
/home/1001/sw/unix-software-dev/src-2//libprintargv/printargv.h
```

- Writing and maintaining Makefiles by hand can become cumbersome
 - A lot of what we embedded in Makefile.inc and Makefile.rules is likely common to almost all projects
 - A lot of what we did by hand could be automated
 - For each source file, determine on what other files it depends (e.g. headers)
 - E.g. gcc ... -MMD ... to emit make-style dependency files
- Compilers (toolchains) have major differences
 - Detect which toolchain is being used, adapt behavior as a result
 - E.g. automatically generate a Makefile.inc to match the build environment
 - o Detect third-party and OS libraries, functions within them, and adapt accordingly
 - Linux printf() behaves differently than Mac OS X printf()

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• The Intel Fortran compiler has different flags versus GCC versus AMD versus

- Solution: provide a higher-level description of what's needed in the build environment, let the computer solve for the variables
 - o GNU autoconf uses configuration files and templates written in the M4 language

```
[frey@login00.darwin src-2]% cd ../src-3
[frey@login00.darwin src-3]% cat configure.ac
AC [NIT([Tutorial Program], 1.0)
AM INIT AITOMAKE
AC PROG CC
AC CONFIG HEADERS([config.h])
AC CONFIG FILES([Makefile])
AC_OUTFUT

[frey@login00.darwin src-3]% autoreconf --install
configure.ac:2: installing './install-sh'
configure.ac:2: installing './install-sh'
configure.ac:2: installing './install-sh'
makefile.am: error: required file './README' not found
Makefile.am: error: required file './README' not found
Makefile.am: error: required file './AuthorS' not found
Makefile.am: error: required file './ChangeLog' not found
Makefile.am: crosi required file './ChangeLog' not found
Makefile.am: crosi required file './ChangeLog' not found
Makefile.am: crosider adding the COFYING found
Makefile.am: for your code, to avoid questions about which license your project uses
Makefile.am: for your code, to avoid questions about which license your project uses
Makefile.am: for your code, to avoid questions about which license your project uses
Makefile.am: installing './depcomp'
autoreconf: automake failed with exit status: 1
```

- Name and version of project in AC_INIT
- AC_PROG_CC activates C language handling
- AC_CONFIG_HEADERS writes automake build environment info as macros to to template config.h.in
- AC_CONFIG_FILES turns a Makefile.am template into template Makefile.in

- Solution: provide a higher-level description of what's needed in the build environment, let the computer solve for the variables
 - o GNU autoconf uses configuration files and templates written in the M4 language

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Generates configure script

- Solution: provide a higher-level description of what's needed in the build environment, let the computer solve for the variables
 - o GNU autoconf uses configuration files and templates written in the M4 language

```
[frey@login00.darwin src-3]6 /configure --help
'configure' configures Tutorial Program 1.0 to adapt to many kinds of systems.

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

To assign environment variables (e.g., CC, FEASS...), 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=recursive display options specific to this package

-help=recursive display the short help of all the included packages

-y. =-vession display version information and exit

-q. =-quiet, =-silent do not print 'checking ...' gessages

-cache-file=FIEIL cache test results in FILE [disabled]

-C. =-config-cache allss for '--cache-file=config-cache'
-n, =-no-create do not create output files

Installation directories:

Installation directories:

install architecture-independent files in FREFIX

[/USF/local]

:
```

- Solution: provide a higher-level description of what's needed in the build environment, let the computer solve for the variables
 - o GNU autoconf uses configuration files and templates written in the M4 language

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• Specify the C compiler to use with the "CC" environment variable

- Solution: provide a higher-level description of what's needed in the build environment, let the computer solve for the variables
 - o GNU autoconf uses configuration files and templates written in the M4 language

```
[frey@login00.darwin build-system] % mkdir ../build-intel ; cd ../build-intel
[frey@login00.darwin build-intel] % tykg_require intel/2020
Adding package 'intel/2020u4' to your environment

[frey@login00.darwin build-intel] % CC=icc ../configure
checking for a BSD-compatible install... /usr/bin/install -c
checking whether build environment is sane... yes

config.status: creating Makefile
config.status: creating config.h
config.status: executing depfiles commands

[frey@login00.darwin build-intel] % make
make all-am
make[1]: Entering directory '/home/1001/sw/unix-software-dev/src-3/build-intel'
icc -DHAVE_CONFIG H -I. -I.. - g-02 -WT printargv.o -MD -MF -MF .deps/printargv.Tpo -c -o printargv.o ../printargv.c

wv -f. deps/printargv.Tpo .deps/printargv.Po
icc -DHAVE_CONFIG H -I. -I.. - g-02 -WT my program.o -MD -MF -MF .deps/my_program.Tpo -c -o my_program.o ../my_program.c

mv -f. deps/my_program.Tpo .deps/my_program.Fo
icc -g -02 -o my_program printargv.o my_program.o
make[1]: Leaving directory '/home/1001/sw/unix-software-dev/src-3/build-intel'
```

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Specify the C compiler to use with the "CC" environment variable

- Solution: provide a higher-level description of what's needed in the build environment, let the computer solve for the variables
 - o GNU autoconf uses configuration files and templates written in the M4 language

```
[frey@login00.darwin build-intel]$ make install
make[l]: Entering directory '/home/1001/sw/unix-software-dev/src-3/build-intel'
/usr/bin/mkdir -p '/usr/local/bin'
/usr/bin/install -c my_program '/usr/local/bin'
/usr/bin/install: cannot create regular file '/usr/local/bin/my_program': Permission denied
make[l]: *** [install-binFROGRAMS] Error 1
make[l]: Leaving directory '/home/1001/sw/unix-software-dev/src-3/build-intel'
make: *** (install-am) Error 2
```

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• Specify the C compiler to use with the "CC" environment variable

- Solution: provide a higher-level description of what's needed in the build environment, let the computer solve for the variables
 - o GNU autoconf uses configuration files and templates written in the M4 language

- The "distclean" target removes the build environment that configure generated
- The —prefix option behaves as our PREFIX variable did back in the previous directory's Makefile infrastructure

- Solution: provide a higher-level description of what's needed in the build environment, let the computer solve for the variables
 - o GNU autoconf uses configuration files and templates written in the M4 language

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 The "distcheck" produces a distributable software package with the configure script and all infrastructure files

- This barely touches on the scope of autoconf
 - o Many resources online not all of them easy to understand
- Main caveat is portability
 - o 100% tied to make build system
 - o Originated on GNU Linux systems
 - Has been ported to other operating systems, but compatibility varies between releases
 - As changes are made to an OS, older autoconf tools may no longer work properly
 - o Changes to compilers, new compilers, must be explicitly handled
 - Newer releases expand coverage of new, sometimes eliminate coverage of old

- To address the issues with autoconf
 - o Use a simpler, more easily-understood language to define build environment
 - o Allow for build systems other than just make
 - o Portable between Linux/Mac/Windows with usage held in common

- To address the issues with autoconf
- Build system description created in CMakeLists.txt files

```
[frey@login00.darwin src-3] cd ../../src-4

[frey@login00.darwin src-4] s ls -1
total 39
-rw-r--r-1 frey everyone 295 Sep 25 17:32 CMakeLists.txt
-rw-r--r-1 frey everyone 113 Sep 25 17:32 my program.c
-rw-r--r-1 frey everyone 185 Sep 25 17:32 printargy.c
-rw-r--r-1 frey everyone 195 Sep 25 17:32 printargy.c
-rw-r--r-1 frey everyone 105 Sep 25 17:32 printargy.h
-rw-r--r-1 frey everyone 105 Sep 25 17:32 printargy.h
-rw-r--r-1 frey everyone 1423 Sep 25 17:32 README.md

[frey@login00.darwin src-4] s cat CMakeLists.txt
cmake_minimum_required (VERSION 2.6)

# Define the project:
project (my_program C)

# The project includes an executable program:
add_executable(my_program my_program.c printargy.c)

# Installation should copy the executable into a "bin" directory:
install (TARGETS my_program DESTINATION bin)
```

- To address the issues with autoconf
- Build system description created in CMakeLists.txt files

```
[frey@login00.darwin src-3] $ cd ../../src-4

[frey@login00.darwin src-4] $ ls -1
total 39
-tw-r--r-1 frey everyone 295 Sep 25 17:32 CMakeLists.txt
-tw-r--r-1 frey everyone 113 Sep 25 17:32 my program.c
-tw-r--r-1 frey everyone 195 Sep 25 17:32 printargy.c
-tw-r--r-1 frey everyone 195 Sep 25 17:32 printargy.c
-tw-r--r-1 frey everyone 105 Sep 25 17:32 printargy.n
-tw-r--r-1 frey everyone 105 Sep 25 17:32 printargy.n
-tw-r--r-1 frey everyone 123 Sep 25 17:32 README.md

[frey@login00.darwin src-4] $ cat CMakeLists txt
cmake_minimum_required (VE

# Define the project:
project (my_program c)

# The project is named "my_program" and uses the C language

# The project includes an executable program:
add_executable(my_program my_program.cprintargv.c)

# Installation should copy the executable into a "bin" directory:
install (TARGETS my_program DESTINATION bin)
```

- To address the issues with autoconf
- Build system description created in CMakeLists.txt files

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- Build system description created in CMakeLists.txt files

- To address the issues with autoconf
- Build system description created in CMakeLists.txt files

```
[frey@login00.darwin src-4]$ mkdir build-system; cd build-system
[frey@login00.darwin build-system]$ vpkg_require cmake/default
Adding package 'cmake/3.21.4' to your environment

[frey@login00.darwin build-system]$ CC=gcc cmake -DCMAKE_INSTALL_PREFIX=/tmp/abc .. :
-- The C compiler identification is GNU 4.8.5
-- Detecting C compiler ABI info - done
-- Detecting C compiler ABI info - done
-- Check for working C compiler: /usr/bin/gcc - skipped
-- Detecting C compile features
-- Detecting C compile features - done
-- Configuring done
-- Generating done
-- Generating done
-- Build files have been written to: /home/1001/sw/unix-software-dev/src-4/build-system

[frey@login00.darwin build-system]$ make
[ 33%] Building C object CMakeFiles/my_program.dir/my_program.c.o
[ 66%] Building C object CMakeFiles/my_program.dir/printargv.c.o
[ 100%] Built target my_program
```

- Interesting naming scheme don't drop the original extension (.c) but append the object extension to it (.c.o)
 - o Preserves some sense of that language the original source was!

- To address the issues with autoconf
- Build system description created in CMakeLists.txt files

```
[frey@login00.darwin build-system]$ rm -rf *; CC=gcc ccmake ..
```

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Build type is used to determine what flags to pass to the compiler for optimization

- To address the issues with autoconf
- Build system description created in CMakeLists.txt files

- To address the issues with autoconf
- Build system description created in CMakeLists.txt files

- Recall the "MD" flag was used to emit dependency rules for the sake of make
 - The "MF" option specifies to what file the rules should be written

- To address the issues with autoconf
- Build system description created in CMakeLists.txt files

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- Multi-directory projects
 - Each directory gets a CMakeLists.txt file defining the build therein
 - Parent directory CMakeLists.txt must reference the sub-directory with the add subdirectory() command
 - Example 5 implements a multi-directory project in CMake v3.x versus the older v2.x language as in Example 4

- 1. Top-level CMakeLists.txt
 - a. **All** compile statements should reference the libprintargv directory for header search
 - b. Both source subdirectories added

- 1. Top-level CMakeLists.txt
- 2. libprintargy
 - a. Create a library target, shared or static based on value of BUILD_SHARED_LIBS variable
 - b. Associate the header file with the target (for the sake of installation)
 - c. Library install destination may vary by system (lib, lib64)

- 1. Top-level CMakeLists.txt
- 2. libprintargv
- 3. my_program
 - a. Create an executable program
 - b. Link the program against the printargy target (defined in libprintargy)

```
# Build an executable:
add_executable(my_program my_program.c)

# The "my_program" target must be linked against the library in
# the "printargy" target that was defined in the libprintargy
# directory:
target_link_libraries (my_program printargy)

# Set the embedded rpath to the installation's library
# directory:
if ( NOT $[CMAKE_SKIP_INSTALL_RPATH ) |
set_target_properties (my_program PROPERTIES |
INSTALL_RFATH $[CMAKE_INSTALL_FULL_LIBDIR])
endif ()

# Installation should copy the executable to the "bin" directory:
install (TARGETS my_program DESTINATION $[CMAKE_INSTALL_BINDIR])
```

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• Build optimized with GCC 12.2, install to /tmp/abc:

```
[frey@login00.darwin ~]$ cd ~/sw/unix-software-dev/src-5

[frey@login00.darwin src-5]$ mkdir build-gcc-12.2; cd build-gcc-12.2

[frey@login00.darwin build-gcc-12.2]$ vpkg_require cmake/default gcc/12.2

Adding package `cmake/3.21.4` to your environment

Adding package `gcc/12.2.0` to your environment

[frey@login00.darwin build-gcc-12.2]$ CC=$(which gcc) cmake -DCMAKE_INSTALL_PREFIX=/tmp/abc -DCMAKE_BUILD_TYPE=Release ..

-- The C compiler identification is GNU 12.2.0

-- Detecting C compiler ABI info

-- Detecting C compiler features

-- Detecting C compiler features

-- Detecting C compile features

-- Detecting
```

• Build optimized with GCC 12.2, install to /tmp/abc:

• Build optimized with GCC 12.2, install to /tmp/abc:

```
[frey@login00.darwin build-gcc-12.2]$ make install
Consolidate compiler generated dependencies of target printargy
[ 50%] Built target printargy
Consolidate compiler generated dependencies of target my_program
[100%] Built target my_program
Install the project...
-- Install configuration: "Release"
-- Installing: /tmp/abc/lib64/libprintargv.so
-- Installing: /tmp/abc/include/printargv.h
-- Installing: /tmp/abc/inmy_program
-- Set runtime path of "/tmp/abc/bin/my_program" to "/tmp/abc/lib64"

[frey@login00.darwin build-gcc-12.2]$ find /tmp/abc
/tmp/abc/lib64
/tmp/abc/lib64/libprintargv.so
/tmp/abc/include
/tmp/abc/include
/tmp/abc/include
/tmp/abc/bin
/tmp/abc/bin
/tmp/abc/bin/my_program
```

• Alternative: do **not** embed "rpath" in the my_program executable

• Alternative: do **not** embed "rpath" in the my program executable

```
[frey@login00.darwin build-gcc-12.2]$ find /tmp/abc /tmp/abc |
/tmp/abc/lib64 |
/tmp/abc/lib64 |
/tmp/abc/include |
/tmp/abc/include |
/tmp/abc/bin |
/tmp/a
```

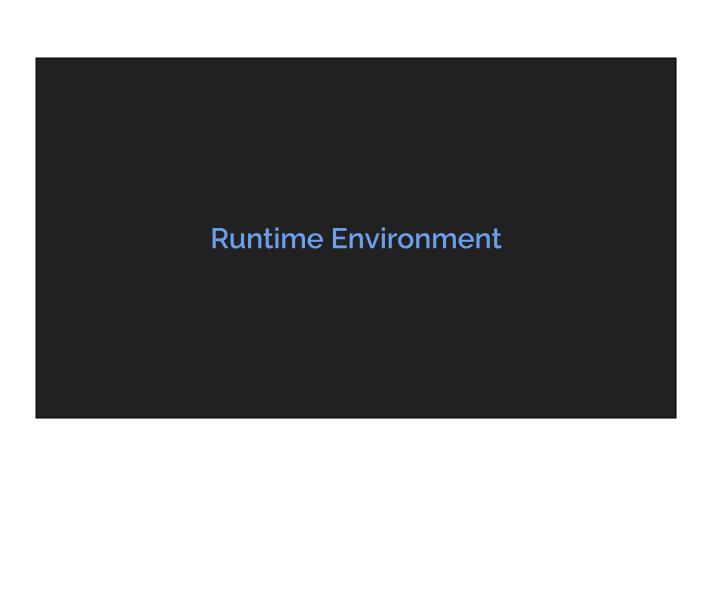
• Alternative: rebuild with debug enabled, use debug library at runtime

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 The executable in /tmp/abc is still the optimized build, but the shared library is a debug build

• Alternative: override embedded library search path at runtime

- Pre-loading brings all of the cited libraries' symbols into memory so that after the executable is loaded NONE are undefined — which would trigger the library search procedure
- Special debugging libraries, for memory management operations for example, are often loaded this way



Runtime Environment

- In Example 5 several environment variables were leveraged
 - PATH: colon-separated list of directories to search for executables
 - LD_LIBRARY_PATH: colon-separated list of directories to search for shared libraries
 - o Others (e.g. MANPATH) provide other search paths

- In Example 5 several environment variables were leveraged
 - o PATH: colon-separated list of directories to search for executables
 - o LD_LIBRARY_PATH: colon-separated list of directories to search for shared libraries
 - Others (e.g. MANPATH) provide other search paths
- Compiled *object code* is assembled into an executable by a *linker*
 - o Resolves named objects (functions, variables) to addresses
 - Addresses may be present in the executable OR a reference to a shared library

- In Example 5 several environment variables were leveraged
 - o PATH: colon-separated list of directories to search for executables
 - o LD_LIBRARY_PATH: colon-separated list of directories to search for shared libraries
 - Others (e.g. MANPATH) provide other search paths
- Compiled *object code* is assembled into an executable by a *linker*
 - o Resolves named objects (functions, variables) to addresses
 - Addresses may be present in the executable OR a reference to a shared library
- When the program is executed, references to shared libraries are resolved by the *runtime linker*
 - o Embedded rpath(s) checked
 - Paths in LD_LIBRARY_PATH checked

- Default paths for installed software components in Linux/Unix
 - o bin: user-accessible executables
 - o sbin: privileged user-accessible executables
 - 0 lib, lib64: shared libraries
 - libexec: helper programs/libraries associated with an executable or library
 - o man, share/man: man pages
 - o include: header files (for software development)
- autoconf and CMake often leverage the same hierarchy for installs
 - Clear categorization of components in both OS and third-party software
 - o Default Linux install prefixes:
 - OS = /usr
 - Add-ons = /usr/local

- Default paths for installed software components in Linux/Unix
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- autoconf and CMake often leverage the same hierarchy for installs
 - Clear categorization of components in both OS and third-party software
 - o Default Linux install prefixes:
 - OS = /usr
 - Add-ons = /usr/local < executable in /usr/local??

How can we install multiple versions/variants of the my_program

- Add a suffix to the my_program name, such as my_program hyphen — v1.0
 - The same suffixing must be used on shared libraries accompanying the program so they can be versioned

- Naming suffixes may not be supported by all software build environments
 - Our projects do not support adding -v1.0 to the executable, library, and header names
- Isolate a version/variant of the software in its own installation root
 - The --prefix option in autoconf; CMAKE INSTALL PATH in CMake
 - o On a Linux system, the components are separated into the usual component paths
 - bin, lib, et al.
- Use a versioned-package hierarchy:
 - < <software-hierarchy>/<package-name>/<version-or-variant-name>
 - $\mathsf{E}.\mathsf{g}$./opt/shared/openmpi/4.1.5-gcc-12.2
 - <software-hierarchy> = /opt/shared
 - <package-name> = openmpi
 - <version-or-variant-name> = 4.1.5-gcc-12.2

- Where will components be found?
 - User executables: /opt/shared/openmpi/4.1.5-gcc-12.2/bir
 - o Libraries: /opt/shared/openmpi/4.1.5-gcc-12.2/lik
 - o Man pages: /opt/shared/openmpi/4.1.5-gcc-12.2/share/man
 - Development headers: /opt/shared/openmpi/4.1.5-gcc-12.2/include
- To use this software, environment variables must be augmented
 - Add respective directories to PATH, LD_LIBRARY_PATH, MANPATH
 - For the sake of development (autoconf, CMake, and others)
 - Add "-I/opt/shared/openmpi/4.1.5-gcc-12.2/include" to CPPFLAGS
 - Add "-L/opt/shared/openmpi/4.1.5-gcc-12.2/lib" to LDFLAGS

- Where will components be found?
 - User executables: /opt/shared/openmpi/4.1.5-gcc-12.2/bir
 - o Libraries: /opt/shared/openmpi/4.1.5-gcc-12.2/lik
 - o Man pages: /opt/shared/openmpi/4.1.5-gcc-12.2/share/man
 - o De
- To use
 - o Ado
 - For
- Many software products will suggest these environment variable changes or other environment alterations should be added to the user's ~/.bashrc or ~/.bash_login file, for example.

Do not follow this advice!

- Why not alter shell login files?
 - Whatever is present in the shell login files affects **every shell** on the cluster
 - Not just your login shell every job shell, too
 - O PATH=/home/1001/sw/pkg/2/bin:/home/1001/sw/pkg/1/bin:...
 - Once you've added version 2, how do you selectively reference version 1?
 - D LD LIBRARY PATH=/home/1001/sw/pkg/2/lib:/home/1001/sw/other pkg/1/lib:..
 - If same library is present in both with e.g. alternative features the runtime linker may not find the correct copy
 - o Python virtual environments (virtualenvs) are particularly bad
 - Many will contain libraries and executables that override what the OS provides
 - In some cases an entire development runtime is embedded (e.g. Ubuntu-style GNU libraries)
 - OS commands may not work with the overriding library versions

P∨t

- Why not alter shell login files?
 - Whatever is present in the shell login files affects **every shell** on the cluster
 - Not just your login shell every job shell, too
 - O PATH=/home/1001/sw/pkg/2/bin:/home/1001/sw/pkg/1/bin:..
 - What's the alternative?

Keep *all* shells as minimally-altered as possible and make changes on-demand, only as necessary to the situation.

When you need to use /home/1001/sw/pkg/1, add its directories to PATH, LD LIBRARY PATH, etc.

OS COMINANAS MAY NOU WORK WITH THE OVERNAING LIDIARY VERSIONS

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untime linker

u-style GNU



- Similar to the popular *modules* environment management
- A package definition file describes environment alterations associated with one or more versions/variants of a package
 - Additions to path, LD LIBRARY PATH, MANPATH
 - Changes to arbitrary environment variables
 - o Define command aliases
 - o Execute (source) shell scripts
 - Load other packages dependencies into the environment, too

- Similar to the popular *modules* environment management
- A package definition file describes environment alterations associated with one or more versions/variants of a package
- How are package definition files found?
 - Default paths:
 - IT RCI managed software: /opt/shared/valet/etc
 - User managed: ~/.valet
 - Value of valet_path behaves like path, Ld_LIBRARY_PATH
 - Added by workgroup: \${WORKDIR}/sw/valet (if the path exists)
 - Users can add their own paths
 - export VALET PATH="/home/1001/sw/valet:\$VALET PATH"

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 By "variants" I mean multiple copies of the same version with different build options — like compiler choice — or with alternative parameterizations

- How are package definition files created?
 - YAML (YAhoo Markup Language) is the preferred format
 - JSON (JavaScript Object Notation) and XML (eXtensible Markup Language) available but not recommended
 - o File should be named <pkg-id>.vpkg yaml
 - o Document is structured with default actions and a dictionary of per-version actions
 - Example presented here is in unix-software-dev/valet-2.1/yaml

- Package-level details
 - The prefix is the directory that contains all versions/variants of the package
 - The actions is a list of alterations to apply to the environment
 - Treat DUMMY_CONF_PATH as a colon-delimited list (like PATH) and add a value to the list
 - The value to add is the etc directory inside the directory containing the version/variant of the package

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• No tabbed whitespace is allowed in YAML, only regular space characters

- Version-level details
 - A version prefix directory can be specified explicitly or it is implied the version id is appended to the package's prefix directory
 - home/1001/sw/dummy/0.1
 - The dependencies is a list of other versioned package ids that are required by this versioned package
 - The dummy program was compiled with GCC 12.2

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- A default version can be explicit or implied
- A version id can have *feature* tags
 - Comma-separated list of strings occurring after a colon
 - Unordered: "a,b,c" == "b,c,a" == "c,a,b"
 - Implicit directory name includes the tags: e.g. 0.1-intel
- A version can be an alternate name for another version id
 - o an alias

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- "I don't see any mention of a bin directory to add to PATH..."
 - VALET automatically checks for standard Linux component directories and adds them to the appropriate environment variables
 - executables, libraries, man pages, etc.
 - Other paths can be explicitly specified
 - Absolute paths
 - Paths relative to the version's prefix directory

```
dummy:

description: Dummy - The software without source or purpose
url: http://www.udel.edu/dummy-software/
prefix: /home/1001/sw/dummy
actions:

- variable: DUMMY_CONF_PATH
action: append-path
value: "$(VALET_PATH_PREFIX)/etc"

default-version: 0.1

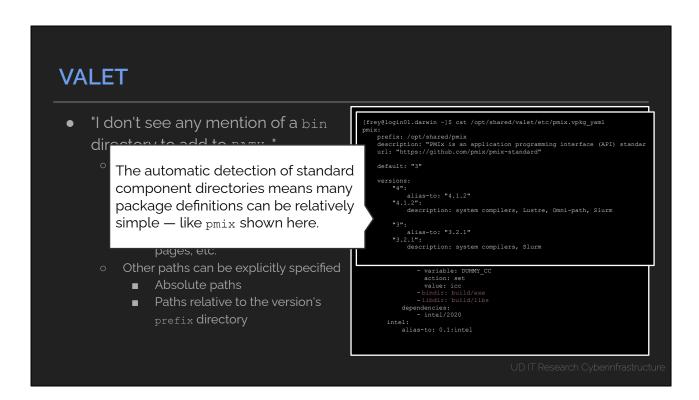
description: Version 0.1 (compiled with GCC 12)
actions:

- variable: DUMMY_CC
action: set
value: gcc
dependencies:
- gcc/12.2

0.1:intel:
description: Version 0.1 (compiled with Intel 2020)
actions:

- variable: DUMMY_CC
action: set
value: gcc
dependencies:
- gcc/12.2

0.1:intel:
description: Version 0.1 (compiled with Intel 2020)
actions:
- variable: DUMMY_CC
action: set
value: icc
- bindir: build/exe
- libdir: build/exe
- libdir: build/libs
dependencies:
- intel/2020
intel:
alias-to: 0.1:intel
```



 It can be very useful to examine the package definition files that IT RCI maintains to gain a better understanding of VALET

- "How do I check if my package definition is valid?"
 - The vpkg_check command validates the file and prints the parsed definition if successful
 - If not successful, information is provided re: at which line the error occurred or what convention was violated
 - Note the implicit prefix directories are displayed
 - Copy/move the file to e.g. ~/.valet to install

- "How do I check what packages are available?"
 - o The vpkg list command
 - Parsable package definitions in each (implicit and explicit) directory have their package id shown

```
[frey@login01.darwin ~] $ vpkg_list

Available packages:
in /home/1001/.valet
dummy
dvipmg
libxc
opencor
vasp
in /opt/shared/valet/2.1/etc
alphafold
amd-rocm
amd-uprof
anaconda
accl
arpack
atlas
autoconf
binutils
blacs
blis
blacs
blis
boost
ccrypt
charm
cmake
colabfold
cryospare
cuda
cudnn
eigen
emacs
fftw
:
```

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- "How do I check what versions or variants of a package are available?"
 - The vpkg versions command

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- "How do I add a versioned package to the environment?"
 - o The vpkg require command
 - The vpkg_devrequire command selects the development context
 - Additional changes are made to
 e.g. CPPFLAGS, LDFLAGS, etc.
- "How do I check what packages have already been added?"
 - o The vpkg history command

```
[frey@login01.darwin ~] $ vpkg_require dummy/intel Adding dependency `intel/2020u4' to your environment Adding package 'dummy/0.1:intel' to your environment

[frey@login01.darwin ~] $ vpkg_history
[standard]
intel/2020u4
dummy/0.1:intel
```

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- "How do I undo the changes made by vpkg_require or vpkg_devreguire commands?"
 - o The vpkg rollback command
 - No arguments = remove the last set of changes
 - Integer argument <*N*> = remove the last <*N*> sets of changes
 - "all" = remove all sets of changes

• "How do I undo the changes

When using $vpkg_devrequire$, each package's prefix directory is added to an environment variable, $<pkg-id>_PREFIX$.

the last <N> sets of changes

■ "all" = remove all sets of changes

```
[frey@login01.darwin ~]$ vpkg_devrequire_udunits/2.2
Adding package `udunits/2.2.28` to your environment

[frey@login01.darwin ~]$ vpkg_history
[standard]
    intel/2020u4
    dummy/0.lintel
[development]
    udunits/2.2.28

[frey@login01.darwin ~]$ echo $CPPFLAGS
-I/opt/shared/udunits/2.2.28/include

[frey@login00.darwin ~]$ echo $UDUNITS_PREFIX
/opt/shared/udunits/2.2.28

[frey@login01.darwin ~]$ vpkg_rollback
[frey@login01.darwin ~]$ vpkg_history
[standard]
    intel/2020u4
    dummy/0.lintel

[frey@login01.darwin ~]$ echo $CPFFLAGS

[frey@login01.darwin ~]$ echo $CPFFLAGS

[frey@login01.darwin ~]$ vpkg_history

[frey@login01.darwin ~]$ vpkg_history
```

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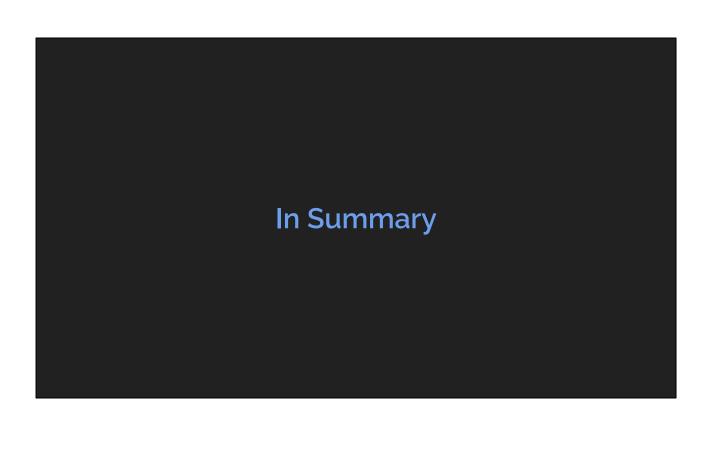
 The prefix variables are very useful in directing autotools and CMake where to find dependencies

- Multiple versioned package ids can be specified in a single command
 - A package's default version is selected with the default version id
 - Any conflicts or errors result in the entire set of changes' being rolled back (not applied)

```
[frey@login01.darwin ~]$ vpkg_require dummyyefault valgrind/3.22.0 r/4.1.3 gcc/11.2.0 conflicts with gcc/12.2.0 already added to environment
```

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- Multiple versioned package ids can be specified in a single command
 - A package's default version is selected with the default version id
 - Any conflicts or errors result in the entire set of changes' being rolled back (not applied)
 - Ignoring conflicts may produce runtime errors!
 - It is always best-practice to minimize the number of sets of changes made to the environment.



- 1. Adopt a hierarchical organization of software
 - 0 <base-dir>/<pkg-name>/<version-or-variant>
 - <base-dir> can be anywhere, but common locations are:
 - <base-dir> = ~/sw (for personally-managed software)
 - <base-dir> = \${WORKDIR}/sw (for software shared by whole workgroup)

- 1. Adopt a hierarchical organization of software
- 2. Adopt the Unix/Linux component directory layout
 - bin.lib.include.share/man.etc.
 - o This often happens by default for software built via autotools or CMake

- 1. Adopt a hierarchical organization of software
- 2. Adopt the Unix/Linux component directory layout
- 3. DO NOT install software by altering login files!
 - .bashrc, .bash profile hands off

- 1. Adopt a hierarchical organization of software
- 2. Adopt the Unix/Linux component directory layout
- 3. DO NOT install software by altering login files!
- 4. Use VALET to manage installed software
 - o If you've followed 1. and 2. then this is much easier!

- 1. Adopt a hierarchical organization of software
- 2. Adopt the Unix/Linux component directory layout
- 3. DO NOT install software by altering login files!
- 4. Use VALET to manage installed software
- 5. When developing software
 - Avoid writing build scripts: autotools, CMake, et al. will always do a better job
 - Relocatable: write software that has no fixed installation directory
 - o Flexible: write software that is configurable at run time, not compile time
 - o Batchable¹: write software that requires **no** interactive input

¹ Yes, I made that word up. Copyright © Jeffrey Frey, 2024.

- 1. Adopt a hierarchical organization of software
- 2. Adopt the Unix/Linux component directory layout
- 3. DO NOT install software by altering login files!
- 4. Use VALET to manage installed software
- 5. When developing software
- 6. Never be afraid to seek help...
 - o ...after you've exhausted other options: web search, documentation