From Ideas to Execution
Building Code on Supercomputers

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building code is complex

- Today's scientists regularly work with "stacks" of code instead of single libraries
  - A minimal "stack" includes MPI and Fortran 77
  - But many of today's applications are frequently more complicated
- We manage complexity with abstractions
  - This is no different when building software

Programming is simply another form of *writing…*

interpreted vs. compiled

- a high level language can be either interpreted or compiled into machine language before being executed on a computer
  - an interpreted program is indirectly executed through an **interpreter**, a separate program that usually runs on the same computer
  - a compiled program is instead translated to machine code by a **compiler** before being executed directly on the computer
- **compiler** - translates a high level language to object code
- **linker** - collects and merges object files into single executables
- **assembler** - assembly -> machine code, **archiver** - static objects -> libraries

Programming is simply another form of *writing ELF binaries*

elf: executable and linkable format

- very simple composition
  - ELF header (architecture, endianness)
  - run-time information (segments)
    - link/load-time information (sections)
    - program data
- tools for examining elf binaries
  - file, nm, ldd, readelf, objdump, patchelf

a basic taxonomy of programming languages

- **machine language** - the native language executed by central processing units on computers, represented usually in hexadecimal
- **assembly language** - an isomorphic mapping between a machine language and a set of human understandable text mnemonics
- **object code**, a collection of separate, named sequences of machine language and associated data and metadata
- **high level language** - a programming languages designed to be abstracted from the specifics of a particular computer architecture
- **scripting language** - a programming language that controls one or more software applications

a basic taxonomy of elf binaries

- **relocatable** - holds code and data suitable for linking with other object files to create an executable or a shared object file (.o)
- **executable** - holds a program suitable for execution
- **shared object file** - holds code and data suitable for linking *either* through the link editor (.so) or the dynamic linker

a brief aside...

who is this?

Rear Admiral Grace Hopper

Famous computer scientist - developer of the first compiler, coined the phrase ‘debug’

Every dependency is implicit until you make it explicit

is code sufficient?

An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.

David Donoho, 1998.

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thirty years ago

“Here’s my .f77 file! I hope you’ve got a computer with 1 MB of RAM…”

ten years ago

“Here’s a bunch of source code and a Makefile, don’t worry I just included all of the dependencies in my code…”

today

"These results rely on a development LAMMPS, an unreleased version of NAMD, a patched version of PETSc, our ported LLVM stack, and the latest commit on this branch from my GitHub repository. Good luck!"

explicit and implicit dependencies

- explicit
  - compilation units (.f, .c, .cxx)
  - external library names
- implicit (by default)
  - header files / template libraries
  - compiler/linker versions, flags, settings
  - external library versions

including vs. linking

- Includes are a pre-processing step in compiling relocatable objects
  - -I flag
    - Directly copies and pastes included files into compilation unit
- Links are references to other relocatable object archives (libfoo.a) or shared object files (libfoo.so)
  - -L flag (Also use the -R flag when linking dynamically)
  - resolved either statically at link-time or dynamically at run-time

building scientific software

- most freely distributed scientific software is designed to be built with make
- **make** [Feldman, 1978] - a software construction tool for building **targets** from their corresponding **dependencies**
  - dependencies are frequently hierarchical (e.g. program: objects: source)
  - builds can be partial (only some **targets** updated) or complete
- the most popular accompanying tool is the GNU build system
  - **GNU build system** [MacKenzie, 1991]- a suite of programming tools for portably building source-code based distributions

how ‘make all’ works

1. look in the current directory for a **Makefile**, a text file containing declarations of targets, their dependencies, and a set of rules for building targets from their respective dependencies

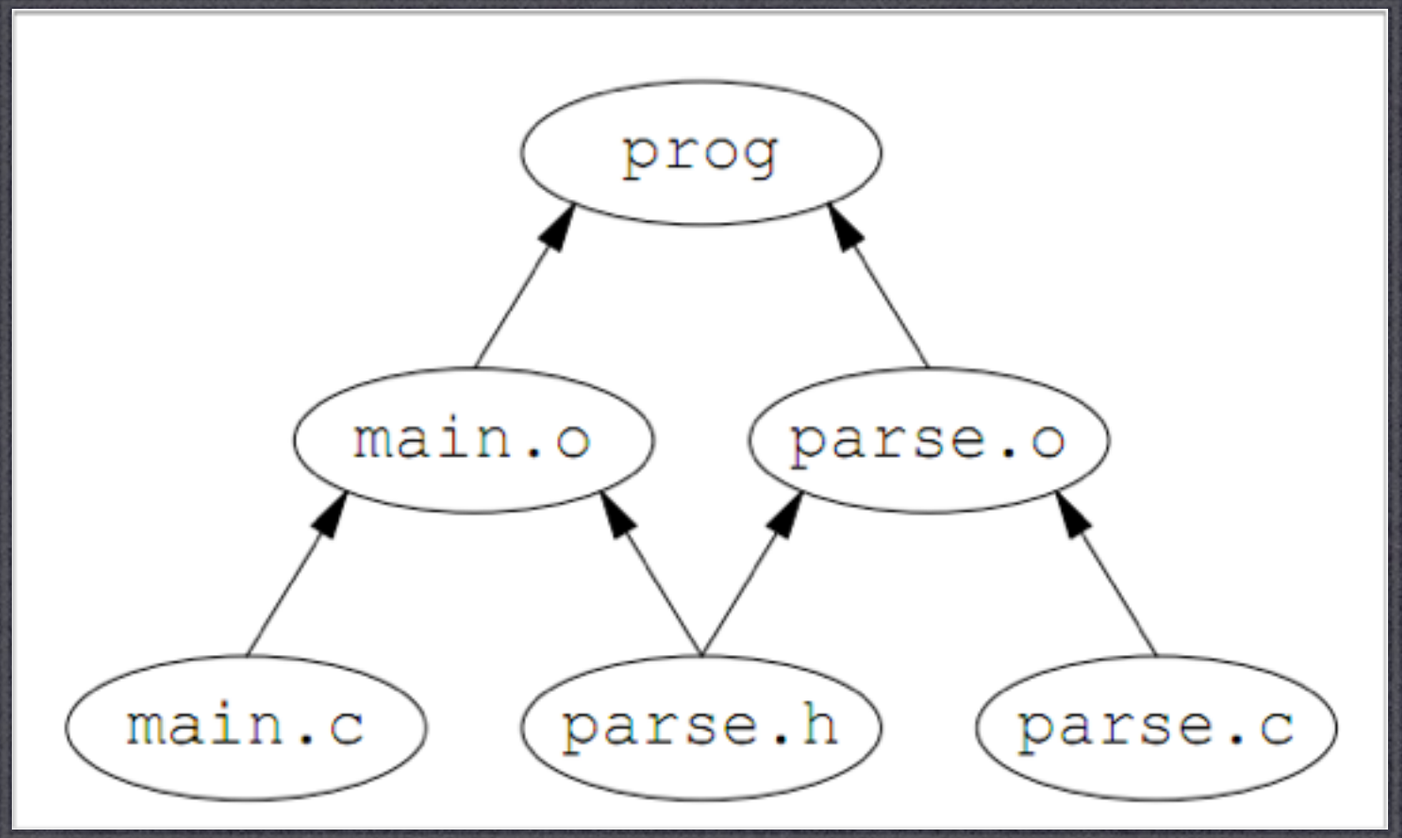
2. construct a directed acyclic graph (DAG) mapping targets to dependencies.

3. traverse the directed acyclic graph and, for each target, find all its dependencies, and update the target if it is older than any of its dependencies (out-of-date)

- a common idiom is to issue make recursively, with a Makefile in each subdirectory of the source tree -- this is often harmful

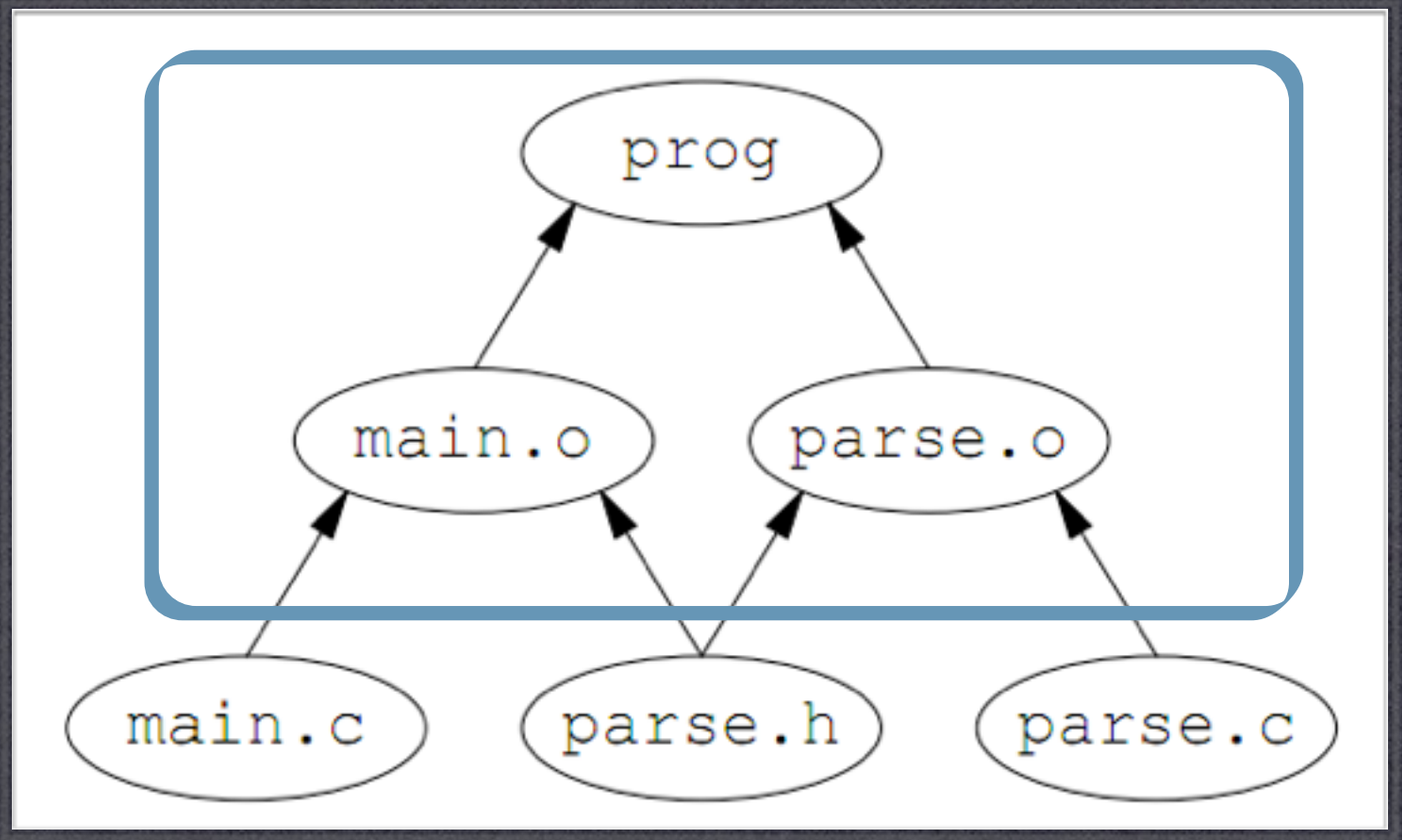
sample makefile/DAG

```
OBJ = main.o parse.o
prog: $(OBJ)
  $(CC) -o $@ $(OBJ)
main.o: main.c parse.h
  $(CC) -c main.c
parse.o: parse.c parse.h
  $(CC) -c parse.c
```



targets

```
OBJ = main.o parse.o
prog: $(OBJ)
  $(CC) -o $@ $(OBJ)
main.o: main.c parse.h
  $(CC) -c main.c
parse.o: parse.c parse.h
  $(CC) -c parse.c
```



dependencies

```
OBJ = main.o parse.o
prog: $(OBJ)
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main.o: main.c parse.h
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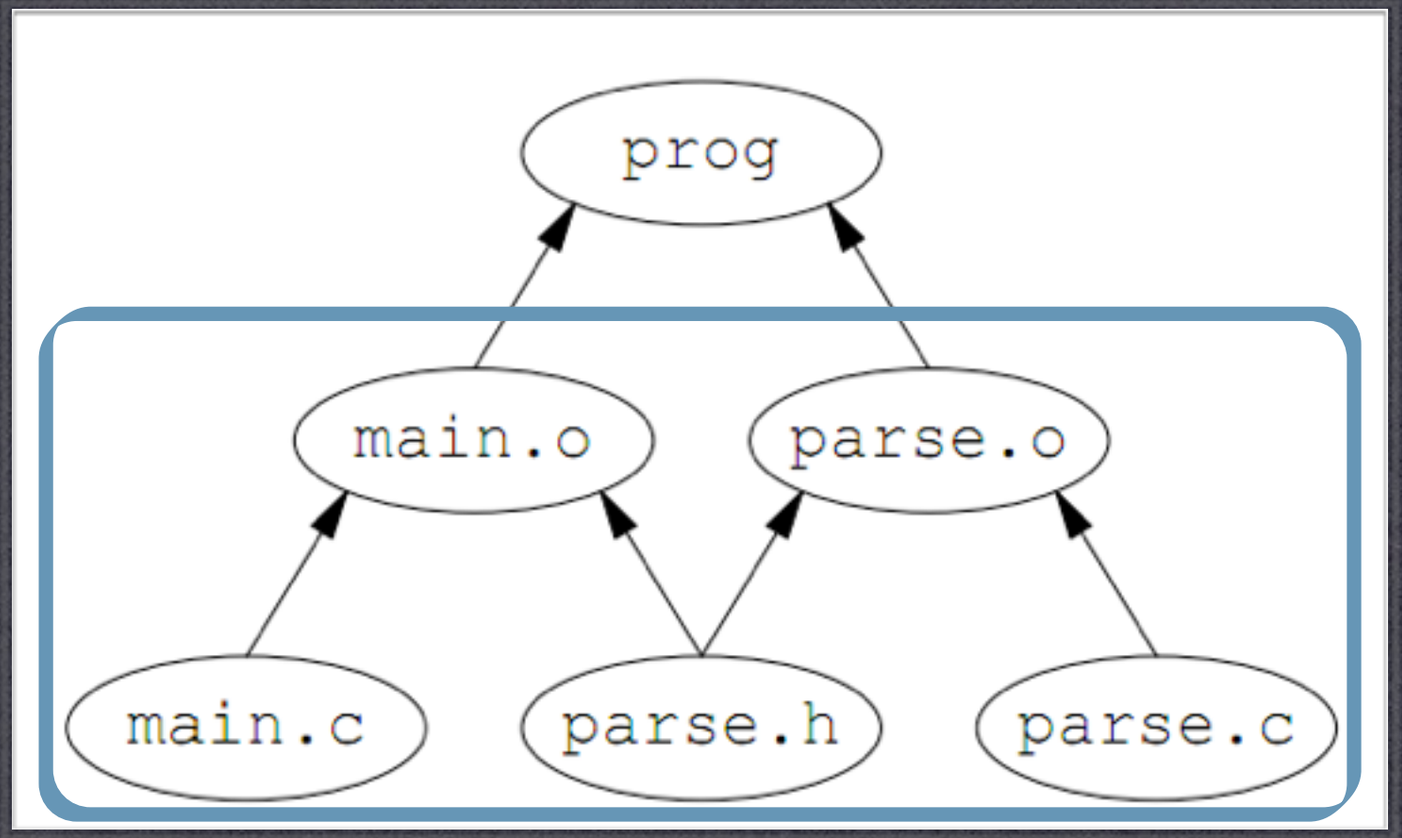

A well designed Makefile can capture a complete scientific workflow

pop quiz: scalability

- assume a makefile with defined *N* targets and *M* independent dependent source files

  - make considers a target to be ‘out-of-date’ when the time stamp of any of its dependencies are more recent than the target

  - what is the minimum number of source files to be considered when evaluating whether to rebuild a single target? all *N* targets?

pop quiz: answers

- how many source files must be considered when evaluating whether to rebuild…
  - single target?

    0. a real target with no dependencies is never rebuilt (but make will still check to see if it exists when you try to build it)

  - all *N* targets?

    all *M* source files must be considered, if any of the dependencies are more recent than their corresponding targets, then the targets must be rebuilt.

deficiencies in standalone make

- doesn't know anything about your system
- cannot determine your dependencies for you
- recursive make can improperly fail to update targets
- scales poorly to very large builds

tools that use make

GNU build system (autoconf, automake, and libtool)	provide configuration, makefile-generation, and library management, implicit dependency tracking
CMake	provides cross-platform configuration and build setup, can generate makefiles in UNIX as well as project files for IDEs such as Visual Studio, implicit dependency scanner

don’t ignore the shell

- Automate with scripts
- Refactor, organize, and control with shell functions
- Manage the build and run context through environment variables
- Use subshells to safely execute commands without modifying the current shell’s working directory or environment variables

Questions?

further reading/sources

- See the previous slides for direct links to the software packages listed
- GNU Make
- [*] Python for Software Design - How to Think Like a Computer Scientist by Allen B. Downey
- [*] Program Library HOWTO by David A. Wheeler
- [*] How to Write Shared Libraries by Ulrich Drepper
- [*] Grace Hopper by Wikipedia Community
- [*] Build System Rules and Algorithms by Mike Shal

photo credits

- Slides 9, 10 (Grace Hopper) from the US Department of the Navy Naval Historical Center, NH 96919-KN, by James S. Davis, 1984

- Slides 20, 21, and 22 (Makefile DAG example) used diagrams lifted from "Recursive Make Considered Harmful", by Peter Miller, 1987