

Lecture 17: Spack an LMod

Software Management with Spack

- Yum installations are precompiled binaries compatible with the core compiler.
- They are usually well tested and stable (good for regular computing)
- The core compiler for a Linux distribution changes only with the Linux version
- Login to Wheeler, Xena, Hopper, and your server and report the core compiler versions for each: `gcc --version`

Software Management with Spack

- In High Performance Computing we usually want to compile our own code:
 1. As we have seen when you compile code for the particular CPU architecture you are using you get performance improvements
 2. We want the freedom to compile with different compilers. You saw that sometimes there is a difference in performance between Intel and GCC compilers.
 3. We want to be able to compile code with the latest fastest compilers.
 4. We might want to modify the source code for programs we deploy
 5. We might want to modify the libraries programs use

Software Management with Spack

- Spack is distributed as a collection of build recipes for thousands of different software packages
- Community based – anyone can submit a new build package
- The packages are written in python so they are easy to modify

Clone the Spack Git Repo into Home Dir

```
[matthew@moonshine spack]$ git clone --depth=100 --  
branch=releases/v0.21 https://github.com/spack/spack.git ~/spack
```

```
[matthew@moonshine spack]$ cd spack
```

```
[matthew@moonshine spack]$ . share/spack/setup-env.sh
```

These are the compilers to which spack has access

```
[matthew@moonshine spack]$ spack compilers
```

We are going to install a new compiler with Spack

```
[matthew@moonshine spack]$ spack list gcc  
armpl-gcc  gcc  gccmakedep  gccxml  
==> 4 packages
```

We are going to install a new compiler with Spack

```
[matthew@moonshine spack]$ spack list gcc  
armpl-gcc  gcc  gccmakedep  gccxml  
==> 4 packages
```

```
[matthew@moonshine spack]$ spack info gcc
```

Description:

The GNU Compiler Collection includes front ends for C, C++, Objective-C, Fortran, Ada, and Go, as well as libraries for these languages.

Homepage: <https://gcc.gnu.org>

Preferred version:

13.2.0 <https://ftpmirror.gnu.org/gcc/gcc-13.2.0/gcc-13.2.0.tar.xz>

Take a look at the gcc package

```
[matthew@moonshine spack]$ spack edit gcc
```

One of the most useful things spack does is handle the many dependencies most HPC software needs.

This is done through simple conditional logic in python.

```
        "RelWithDebInfo: -O2 -g; MinSizeRel: -Os",
    )
    variant(
        "profiled",
        default=False,
        description="Use Profile Guided Optimization",
        when="+bootstrap %gcc",
    )

    depends_on("flex", type="build", when="@master")

    # https://gcc.gnu.org/install/prerequisites.html
    depends_on("gmp@4.3.2:")
    # mawk is not sufficient for go support
    depends_on("gawk@3.1.5:", type="build")
    depends_on("texinfo@4.7:", type="build")
    depends_on("libtool", type="build")
    # dependencies required for git versions
    depends_on("m4@1.4.6:", when="@master", type="build")
    depends_on("automake@1.15.1:", when="@master", type="build")
    depends_on("autoconf@2.69:", when="@master", type="build")

    depends_on("gmake@3.80:", type="build")
    depends_on("perl@5", type="build")

    # GCC 7.3 does not compile with newer releases on some platforms, see
    # https://github.com/spack/spack/issues/6902#issuecomment-433030376
    depends_on("mpfr@2.4.2:3.1.6", when="@:9.9")
    depends_on("mpfr@3.1.0:", when="@10:")
    depends_on("mpc@1.0.1:", when="@4.5:")
    # Already released GCC versions do not support any newer version of ISL
    # GCC 5.4 https://github.com/spack/spack/issues/6902#issuecomment-433072097
    # GCC 7.3 https://github.com/spack/spack/issues/6902#issuecomment-433030376
    # GCC 9+ https://gcc.gnu.org/bugzilla/show_bug.cgi?id=86724
```

Spack generates a dependency tree

```
[matthew@moonshine spack]$ spack spec gcc
```

Concretized

```
-----  
- gcc@13.2.0%gcc@12.3.0~binutils+bootstrap~graphite~nvptx~piclibs~profiled~strip build_system=autotools build_type=RelWithDebInfo languages=c,c++,f  
andybridge  
[+] ^diffutils@3.9%gcc@12.3.0 build_system=autotools arch=linux-rocky9-sandybridge  
[+] ^libiconv@1.17%gcc@12.3.0 build_system=autotools libs=shared,static arch=linux-rocky9-sandybridge  
- ^gawk@5.2.2%gcc@12.3.0~nls build_system=autotools arch=linux-rocky9-sandybridge  
[+] ^libsigsegv@2.14%gcc@12.3.0 build_system=autotools arch=linux-rocky9-sandybridge  
[+] ^readline@8.2%gcc@12.3.0 build_system=autotools patches=bbf97f1 arch=linux-rocky9-sandybridge  
[+] ^gmake@4.4.1%gcc@12.3.0~guile build_system=generic arch=linux-rocky9-sandybridge  
- ^gmp@6.2.1%gcc@12.3.0+cxx build_system=autotools libs=shared,static patches=69ad2e2 arch=linux-rocky9-sandybridge  
[+] ^autoconf@2.69%gcc@12.3.0 build_system=autotools patches=35c4492,7793209,a49dd5b arch=linux-rocky9-sandybridge  
[+] ^automake@1.16.5%gcc@12.3.0 build_system=autotools arch=linux-rocky9-sandybridge  
[+] ^m4@1.4.19%gcc@12.3.0+sigsegv build_system=autotools patches=9dc5fbd,bfdffa7 arch=linux-rocky9-sandybridge  
[+] ^libtool@2.4.7%gcc@12.3.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^mpc@1.3.1%gcc@12.3.0 build_system=autotools libs=shared,static arch=linux-rocky9-sandybridge  
- ^mpfr@4.2.0%gcc@12.3.0 build_system=autotools libs=shared,static arch=linux-rocky9-sandybridge  
- ^autoconf-archive@2023.02.20%gcc@12.3.0 build_system=autotools arch=linux-rocky9-sandybridge  
[+] ^perl@5.38.0%gcc@12.3.0+cpanm+opcode+open+shared+threads build_system=generic patches=714e4d1 arch=linux-rocky9-sandybridge  
[+] ^berkeley-db@18.1.40%gcc@12.3.0+cxx~docs+stl build_system=autotools patches=26090f4,b231fcc arch=linux-rocky9-sandybridge  
[+] ^bzip2@1.0.8%gcc@12.3.0~debug~pic+shared build_system=generic arch=linux-rocky9-sandybridge  
[+] ^gdbm@1.23%gcc@12.3.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^texinfo@7.0.3%gcc@12.3.0 build_system=autotools arch=linux-rocky9-sandybridge  
[+] ^gettext@0.22.3%gcc@12.3.0+bzip2+curses+git~libunistring+libxml2+pic+shared+tar+xz build_system=autotools arch=linux-rocky9-sandybridge  
[+] ^libxml2@2.10.3%gcc@12.3.0+pic~python+shared build_system=autotools arch=linux-rocky9-sandybridge  
[+] ^tar@1.34%gcc@12.3.0 build_system=autotools zip=pigz arch=linux-rocky9-sandybridge  
[+] ^pigz@2.7%gcc@12.3.0 build_system=makefile arch=linux-rocky9-sandybridge  
[+] ^xz@5.4.1%gcc@12.3.0~pic build_system=autotools libs=shared,static arch=linux-rocky9-sandybridge  
[+] ^ncurses@6.4%gcc@12.3.0~symlinks+termlib abi=none build_system=autotools arch=linux-rocky9-sandybridge  
[+] ^pkgconf@1.9.5%gcc@12.3.0 build_system=autotools arch=linux-rocky9-sandybridge  
[+] ^zlib-ng@2.1.4%gcc@12.3.0+compat+opt build_system=autotools arch=linux-rocky9-sandybridge  
[+] ^zstd@1.5.5%gcc@12.3.0+programs build_system=makefile compression=none libs=shared,static arch=linux-rocky9-sandybridge
```

We are going to install a new compiler with Spack

```
[matthew@moonshine spack]$ spack install gcc  
/home/matthew/spack/opt/spack/linux-rocky9-sandybridge/
```

```
[matthew@moonshine spack]$ spack find gcc
```

```
[matthew@moonshine spack]$ spack load gcc@13
```

```
[matthew@moonshine spack]$ spack compiler find
```

```
[matthew@moonshine spack]$ spack compilers
```

We are going to install a new compiler with Spack

```
[matthew@moonshine spack]$ spack find gcc
```

```
-- linux-rocky9-sandybridge / gcc@12.3.0 -----  
-----
```

```
gcc@13.2.0
```

```
[matthew@moonshine spack]$ spack load gcc@13
```

We are going to install a new compiler with Spack

```
[matthew@moonshine spack]$ spack compiler find
```

```
==> Added 1 new compiler to  
/home/matthew/.spack/linux/compilers.yaml
```

```
gcc@13.2.0
```

```
==> Compilers are defined in the following files:  
/home/matthew/.spack/linux/compilers.yaml
```

We are going to install a new compiler with Spack

```
[matthew@moonshine spack]$ spack compilers
```

```
==> Available compilers
```

```
-- gcc rocky9-x86_64 -----
```

```
gcc@13.2.0    gcc@11.4.1
```



The LINPACK Benchmark: Past, Present, and Future*

Jack J. Dongarra[†], Piotr Luszczek[‡], and Antoine Petitet[‡]

July 2002

Abstract

This paper describes the LINPACK Benchmark [41] and some of its variations commonly used to assess performance of computer systems. Aside from the LINPACK benchmark suite, the TOP500 [43], and the HPL [48] code are presented. The latter is frequently used to obtain results for TOP500 submissions. Information is also given on how to interpret results of the benchmark and how the results fit into performance evaluation process.

Keywords: BLAS, benchmarking, high performance computing, HPL, linear algebra, LINPACK, TOP500

1 Introduction

The original LINPACK Benchmark is, in some sense, an accident. It was originally designed to assist users of the LINPACK package [15] by providing information on execution times required to solve a system of linear equations. The first “LINPACK Benchmark” report appeared as an appendix in the LINPACK Users’ Guide [15] in 1979. The appendix comprised of data for one commonly used path in the LINPACK software package. Results were provided for a matrix problem of size 100, on a collection of widely used computers (23 computers in all). This was done so users could estimate the time required to solve their matrix problem by extrapolation.

Jack Dongarra
(Far left)



New Mexico

Clev Moler's PhD
Student

Installing the High Performance Linpack Benchmark

- `[matthew@moonshine spack]$ spack info hpl`
- `AutotoolsPackage: hpl`
-
- `Description:`
 - HPL is a software package that solves a (random) dense linear system in double precision (64 bits) arithmetic on distributed-memory computers.
 - It can thus be regarded as a portable as well as freely available implementation of the High Performance Computing Linpack Benchmark.
 -
- `Homepage: https://www.netlib.org/benchmark/hpl/`
-
- `Preferred version:`
 - `2.3 https://www.netlib.org/benchmark/hpl/hpl-2.3.tar.gz`

Installing the High Performance Linpack Benchmark

```
[matthew@moonshine spack]$ spack spec hpl %gcc@13
```

Concretized

```
-----  
- hpl@2.3%gcc@13.2.0~openmp build_system=autotools arch=linux-rocky9-sandybridge  
- ^gmake@4.4.1%gcc@13.2.0~guile build_system=generic arch=linux-rocky9-sandybridge  
- ^openblas@0.3.24%gcc@13.2.0~bignuma~consistent_fpcsr+fortran~ilp64+locking+pic+shared build_system=makefile symbol_suffix=none threads=none arch=linux-rocky9-sandybrid  
ge  
- ^perl@5.38.0%gcc@13.2.0+cpanm+opcode+open+shared+threads build_system=generic patches=714e4d1 arch=linux-rocky9-sandybridge  
- ^berkeley-db@18.1.40%gcc@13.2.0+cxx~docs+stl build_system=autotools patches=26090f4,b231fcc arch=linux-rocky9-sandybridge  
- ^bzip2@1.0.8%gcc@13.2.0~debug~pic+shared build_system=generic arch=linux-rocky9-sandybridge  
- ^diffutils@3.9%gcc@13.2.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^gdbm@1.23%gcc@13.2.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^readline@8.2%gcc@13.2.0 build_system=autotools patches=bbf97f1 arch=linux-rocky9-sandybridge  
- ^openmpi@4.1.6%gcc@13.2.0~atomics~cuda~cxx~cxx_exceptions~gpfs~internal-hwloc~internal-pmix~java~legacylaunchers~lustre~memchecker~openshmem~orterunprefix+romio+rsh~si  
ngularity+static+vt+wrapper-rpath build_system=autotools fabrics=none schedulers=none arch=linux-rocky9-sandybridge  
- ^hwloc@2.9.1%gcc@13.2.0~cairo~cuda~gl~libudev+libxml2~netloc~nvml~oneapi-level-zero~opencl+pci~rocm build_system=autotools libs=shared,static arch=linux-rocky9-san  
dybridge  
- ^libpciaccess@0.17%gcc@13.2.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^util-macros@1.19.3%gcc@13.2.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^libxml2@2.10.3%gcc@13.2.0+pic~python+shared build_system=autotools arch=linux-rocky9-sandybridge  
- ^libiconv@1.17%gcc@13.2.0 build_system=autotools libs=shared,static arch=linux-rocky9-sandybridge  
- ^xz@5.4.1%gcc@13.2.0~pic build_system=autotools libs=shared,static arch=linux-rocky9-sandybridge  
- ^ncurses@6.4%gcc@13.2.0~symlinks+termlib abi=none build_system=autotools arch=linux-rocky9-sandybridge  
- ^numactl@2.0.14%gcc@13.2.0 build_system=autotools patches=4e1d78c,62fc8a8,ff37630 arch=linux-rocky9-sandybridge  
- ^autoconf@2.69%gcc@13.2.0 build_system=autotools patches=35c4492,7793209,a49dd5b arch=linux-rocky9-sandybridge  
- ^automake@1.16.5%gcc@13.2.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^libtool@2.4.7%gcc@13.2.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^m4@1.4.19%gcc@13.2.0+sigsegv build_system=autotools patches=9dc5fbd,bfdffa7 arch=linux-rocky9-sandybridge  
- ^libsigsegv@2.14%gcc@13.2.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^openssh@9.5p1%gcc@13.2.0+gssapi build_system=autotools arch=linux-rocky9-sandybridge  
- ^krb5@1.20.1%gcc@13.2.0+shared build_system=autotools arch=linux-rocky9-sandybridge  
- ^bison@3.8.2%gcc@13.2.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^findutils@4.9.0%gcc@13.2.0 build_system=autotools patches=440b954 arch=linux-rocky9-sandybridge  
- ^gettext@0.22.3%gcc@13.2.0+bzip2+curses+git~libunistring+libxml2+pic+shared+tar+xz build_system=autotools arch=linux-rocky9-sandybridge  
- ^tar@1.34%gcc@13.2.0 build_system=autotools zip=pigz arch=linux-rocky9-sandybridge  
- ^pigz@2.7%gcc@13.2.0 build_system=makefile arch=linux-rocky9-sandybridge  
- ^zstd@1.5.5%gcc@13.2.0+programs build_system=makefile compression=none libs=shared,static arch=linux-rocky9-sandybridge  
- ^libedit@3.1-20210216%gcc@13.2.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^libxcrypt@4.4.35%gcc@13.2.0~obsolete_api build_system=autotools patches=4885da3 arch=linux-rocky9-sandybridge  
- ^openssl@3.1.3%gcc@13.2.0~docs+shared build_system=generic certs=mozilla arch=linux-rocky9-sandybridge  
- ^ca-certificates-mozilla@2023-05-30%gcc@13.2.0 build_system=generic arch=linux-rocky9-sandybridge  
- ^pkgconf@1.9.5%gcc@13.2.0 build_system=autotools arch=linux-rocky9-sandybridge  
- ^pmix@5.0.1%gcc@13.2.0~docs+pmi_backwards_compatibility~python~restful build_system=autotools arch=linux-rocky9-sandybridge  
- ^libevent@2.1.12%gcc@13.2.0+openssl build_system=autotools arch=linux-rocky9-sandybridge  
- ^zlib-ng@2.1.4%gcc@13.2.0+compat+opt build_system=autotools arch=linux-rocky9-sandybridge
```

Installing the High Performance Linpack Benchmark

```
[matthew@moonshine spack]$ spack install hpl %gcc@13
```

```
==> Installing gmake-4.4.1-ufqig5vxmfp4j7cdu3trou5sxsnk3ire [1/39]
```

```
==> No binary for gmake-4.4.1-ufqig5vxmfp4j7cdu3trou5sxsnk3ire found: installing from source
```

```
==> Using cached archive: /home/matthew/spack/var/spack/cache/source-cache/archive/dd/dd16fb1d67bfab79a72f5e8390735c49e3e8e70b4945a15ab1f81ddb78658fb3.tar.gz
```

```
==> No patches needed for gmake
```

```
==> gmake: Executing phase: 'install'
```

```
==> gmake: Successfully installed gmake-4.4.1-ufqig5vxmfp4j7cdu3trou5sxsnk3ire
```

```
Stage: 0.09s. Install: 17.88s. Post-install: 0.03s. Total: 18.03s
```

```
[+] /home/matthew/spack/opt/spack/linux-rocky9-sandybridge/gcc-13.2.0/gmake-4.4.1-ufqig5vxmfp4j7cdu3trou5sxsnk3ire
```

```
==> Installing ca-certificates-mozilla-2023-05-30-i3umzs4ore6nnlyxhuezcebzcc5zo3ow [2/39]
```

```
==> No binary for ca-certificates-mozilla-2023-05-30-i3umzs4ore6nnlyxhuezcebzcc5zo3ow found: installing from source
```

```
==> Using cached archive: /home/matthew/spack/var/spack/cache/source-cache/archive/5f/5fadcae90aa4ae041150f8e2d26c37d980522cdb49f923fc1e1b5eb8d74e71ad
```

```
==> No patches needed for ca-certificates-mozilla
```

```
==> ca-certificates-mozilla: Executing phase: 'install'
```

```
==> ca-certificates-mozilla: Successfully installed ca-certificates-mozilla-2023-05-30-i3umzs4ore6nnlyxhuezcebzcc5zo3ow
```

```
Stage: 0.00s. Install: 0.00s. Post-install: 0.03s. Total: 0.06s
```



Install the Lmod system

```
sudo yum install lua lua-devel lua-json lua-lpeg lua-posix lua-term tcl  
tcl-devel bc  
git clone https://github.com/TACC/Lmod.git  
cd Lmod/  
./configure --prefix=/opt/  
sudo make install  
sudo ln -s /opt/lmod/lmod/init/profile /etc/profile.d/z00_lmod.sh
```