

Mastering Spack: Managing HPC Software and Dependencies with Precision

In previous article titled "The HPC Software Stack: Spack + Conda + Singularity for Reproducible and Portable Workflows", it introduced a high-level view of how these three powerful tools can be combined to build reproducible and portable HPC workflows. That article emphasized the why - the need for isolated, shareable environments in scientific computing. This follow-up article focuses on the how, starting with Spack - a flexible, compiler and architecture-aware package manager purpose-built for high-performance computing environments. Spack excels in situations where researchers need

- Multiple versions of the same library
- Tight control over compiler and architecture options
- Complex dependency trees with fine-tuned variants

This article will walk through how to use Spack in practical HPC scenarios which not only covers basic usage but also advanced features like variant flags, compiler targeting, dependency chaining, etc. This article explores how to install a complex, real-world application: LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator), a widely-used classical molecular dynamics code with specific variants (like MPI, OpenMP, and GPU support), control compilers, specifying dependency versions and features.

A) Exploring the LAMMPS Package in spack

Load the spack module

```
[user@login1 ~] $ module load spack/spack
```

Get Information about lammps package available in spack repository.

```
[user@login1 ~] $ spack info lammps
```

Once this command is executed, it will fetch all details related to LAMMPS package like available versions, variants(mpi, openmpi, cuda, etc.), build and runtime dependencies, etc.

B) To build Lammps with openmpi support and having rigid and manybody package enabled.

To install LAMMPS version 20220324

```
[user@login1 ~] $ spack install lammps@20240829 +mpi +rigid +manybody +openmp ^openmpi
```

→ To use specific variants of package

→ Control compiler

Here, using '@' means to install specific version, '+' means include or enable the package or variant and '^' and '%' are used to update the package which is directly/indirectly used as a dependency for root package. To include GPU support, user may add +cuda cuda_arch=11

The spack will start building the consistent Dependency Graph related to mentioned versions in the installation command, and if the build is successful, the installation process will start.

```
[testuser2@login1 ~]$ spack install lammps@20240829 +mpi +rigid +manybody +openmp ^openmpi
[+] /usr (external glibc-2.17-7wxodechzwx45ns2cupxtw2w6k2abyv)
==> Installing gcc-runtime-4.8.5-wtvlpinmrcgekcxdbgyzyanc5kaznqc [2/44]
==> No binary for gcc-runtime-4.8.5-wtvlpinmrcgekcxdbgyzyanc5kaznqc found: installing from source
==> No patches needed for gcc-runtime
==> gcc-runtime: Executing phase: 'install'
==> gcc-runtime: Successfully installed gcc-runtime-4.8.5-wtvlpinmrcgekcxdbgyzyanc5kaznqc
Stage: 0.00s. Install: 0.82s. Post-install: 0.03s. Total: 0.91s
[+] /home/testuser2/.spack/opt/spack/linux-rhel7-haswell/gcc-4.8.5/gcc-runtime-4.8.5-wtvlpinmrcgekcxdbgyzyanc5kaznqc
==> Installing ca-certificates-mozilla-2023-05-30-5avwvbf7glw5iukibzk7o3bcvc3otli [3/44]
==> No binary for ca-certificates-mozilla-2023-05-30-5avwvbf7glw5iukibzk7o3bcvc3otli found: installing from source
==> Fetching https://mirror.spack.io/_source-cache/archive/5f/5fadcae90aa4ae041150f8e2d26c37d980522cdb49f923fc1e1b5eb
==> No patches needed for ca-certificates-mozilla
==> ca-certificates-mozilla: Executing phase: 'install'
==> ca-certificates-mozilla: Successfully installed ca-certificates-mozilla-2023-05-30-5avwvbf7glw5iukibzk7o3bcvc3otli
Stage: 0.14s. Install: 0.00s. Post-install: 0.01s. Total: 0.23s
[+] /home/testuser2/.spack/opt/spack/linux-rhel7-haswell/gcc-4.8.5/ca-certificates-mozilla-2023-05-30-5avwvbf7glw5iukibzk7o3bcvc3otli
==> Installing gmake-4.4.1-f4vnz6sujvq3qyr5mt2goehgxisekapl [4/44]
==> No binary for gmake-4.4.1-f4vnz6sujvq3qyr5mt2goehgxisekapl found: installing from source
==> Fetching https://mirror.spack.io/_source-cache/archive/dd/dd16fb1d67bfab79a72f5e8390735c49e3e8e70b4945a15ab1f81dd
==> No patches needed for gmake
==> gmake: Executing phase: 'install'
==> gmake: Successfully installed gmake-4.4.1-f4vnz6sujvq3qyr5mt2goehgxisekapl
Stage: 0.60s. Install: 23.76s. Post-install: 0.02s. Total: 24.46s
[+] /home/testuser2/.spack/opt/spack/linux-rhel7-haswell/gcc-4.8.5/gmake-4.4.1-f4vnz6sujvq3qyr5mt2goehgxisekapl
==> Installing util-macros-1.20.1-sh3ydxh36lqevicirckn6bwn6ilh2xjy [5/44]
```

C) To view the Dependency Tree before installing (Optional)**# To view Dependency Tree**

```
[user@login1 ~] $ spack spec lammps@20240829 +mpi +rigid +manybody +openmp ^openmpi
```

```
[testuser2@login1 ~]$ spack spec lammps@20240829 +mpi +rigid +manybody +openmp ^openmpi
==> Fetching https://mirror.spack.io/bootstrap/github-actions/v0.5/build_cache/linux-centos7-x86_64-gcc-10.2.1-clingo-bootstrap-spack-zowwoa
==> Fetching https://mirror.spack.io/bootstrap/github-actions/v0.5/build_cache/linux-centos7-x86_64-gcc-10.2.1/clingo-bootstrap-spack/linux-
owwoarrf3hvo6i3iereolfujr42iyyro.spack
==> Installing "clingo-bootstrap@=spack%gcc@=10.2.1~docs+ipo+optimized+python+static_libstdcpp build_system=cmake build_type=Release generat
-x86_64" from a buildcache
- lammps@20240829.1%gcc@4.8.5~adios~amoeba~asphere~atc~awpmd~bocs~body~bpm~brownian~cg-dna~cg-spica~class2~colloid~colvars~compress~cores
ole~dpd~basic~dpd~meso~dpd~react~dpd~smooth~drude~eff~electrode~extra~compute~extra~dump~extra~fix~extra~molecule~extra~pair~fep~ffmpeg~gran
kos~kspace~latboltz~lepton~lib~machdyn~manifold~manybody~mc~meam~mesont~mgpt~misc~ml~hdnnp~ml~iap~ml~pod~ml~rann~ml~snap~ml~uf3~mofff~molecu
~opt~orient~peri~phonon~plugin~plumed~png~poems~ptm~python~qeq~qtb~reaction~reaxff~replica~rheo~rigid~rocm~shock~smtbq~sph~spin~srd~tally~to
type=Release fft=fftw3 fftw_precision=double generator=make gpu_precision=mixed lammps_sizes=smallbig arch=linux-rhel7-haswell
- ^cmake@3.30.5%gcc@4.8.5~doc~ncurses~ownlibs~qtgui build_system=generic build_type=Release patches=dbc3892 arch=linux-rhel7-haswell
- ^curl@8.10.1%gcc@4.8.5~gssapi~ldap~libidn2~librtmp~libssh~libssh2~nghttp2 build_system=autotools libs=shared,static tls=openssl
- ^nghttp2@1.63.0%gcc@4.8.5 build_system=autotools arch=linux-rhel7-haswell
- ^diffutils@3.10%gcc@4.8.5 build_system=autotools arch=linux-rhel7-haswell
- ^openssl@3.4.0%gcc@4.8.5~docs~shared build_system=generic certs=mozilla arch=linux-rhel7-haswell
- ^ca-certificates~mozilla@2023-05-30%gcc@4.8.5 build_system=generic arch=linux-rhel7-haswell
- ^ncurses@6.5%gcc@4.8.5~symlinks~term~abi=none build_system=autotools patches=7a351bc arch=linux-rhel7-haswell
- ^zlib-ng@2.2.1%gcc@4.8.5~compat~new_strategies~opt~pic~shared build_system=autotools arch=linux-rhel7-haswell
- ^fftw@3.3.10%gcc@4.8.5~mpi~openmp~pfft~patches~shared build_system=autotools patches=872cff9 precision=double,float arch=linux-rhel
- ^gcc-runtime@4.8.5%gcc@4.8.5 build_system=generic arch=linux-rhel7-haswell
[e] ^glibc@2.17%gcc@4.8.5 build_system=autotools patches=be65fec,e179c43 arch=linux-rhel7-haswell
- ^make@4.4.1%gcc@4.8.5~guile build_system=generic arch=linux-rhel7-haswell
- ^openmpi@5.0.5%gcc@4.8.5~atomics~cuda~debug~goms~internal~hwloc~internal~libevent~internal~rmix~java~lustre~memchecker~opendshmem~ro
```

D) To check whether the package is installed or not**# To check whether lammps is installed or not along with all the dependencies**

```
[user@login1 ~] $ spack find -ldf lammps
```

```
[testuser2@login1 ~]$ spack find -ldf lammps
-- linux-rhel7-haswell / gcc@4.8.5 -----
ysxyfay lammps@20240829.1%gcc
jsjt4m6 cmake@3.30.5%gcc
57hjaol curl@8.10.1%gcc
2ze3eu3 nghttp2@1.63.0%gcc
yllicrsu diffutils@3.10%gcc
3fz2z2s3 openssl@3.4.0%gcc
5avvybhh ca-certificates~mozilla@2023-05-30%gcc
gtdawvf ncurses@6.5%gcc
1712lbf zlib-ng@2.2.1%gcc
4acd6fi fftw@3.3.10%gcc
wtvlpin gcc-runtime@4.8.5%gcc
7wxodec glibc@2.17%gcc
f4vz6s gmake@4.4.1%gcc
12t372c openmpi@5.0.5%gcc
dd6e7x2 autoconf@2.72%gcc
46bd652 m4@1.4.19%gcc
5odacnw libsigsegv@2.14%gcc
3ustuo3 automake@1.16.5%gcc
t7f7vx7 hwloc@2.11.1%gcc
wusiw2i libpciaccess@0.17%gcc
sh3ydxh util-macros@1.20.1%gcc
3mjvchq libxml2@2.13.4%gcc
kx273a7 xz@5.4.6%gcc
udmjgz6 libevent@2.1.12%gcc
bz3rxz2 libtool@2.4.7%gcc
2djyc2n findutils@4.9.0%gcc
zbnhivs numactl@2.0.18%gcc
gxxygde openssh@9.9p1%gcc
ykl4a6u krb5@1.21.3%gcc
rx53sdy bison@3.8.2%gcc
jtf7rn5p gettext@0.21.1%gcc
htshowj tar@1.34%gcc
3wh3ndb pigz@2.8%gcc
wqv7t6h zstd@1.5.6%gcc
l1p2d7g libedit@3.1-20240808%gcc
csmvjpp libxcrypt@4.4.35%gcc
s6nlfwv perl@5.40.0%gcc
lygnc65 berkeley-db@18.1.40%gcc
cm3bngx bzip2@1.0.8%gcc
s3wmb3g gdbm@1.23%gcc
tnefa27 readline@8.2%gcc
nvchxvc pkgconf@2.2.0%gcc
pkate3z pmix@5.0.3%gcc

==> 1 installed package
```

E) To use the installed LAMMPS package and run the example input script

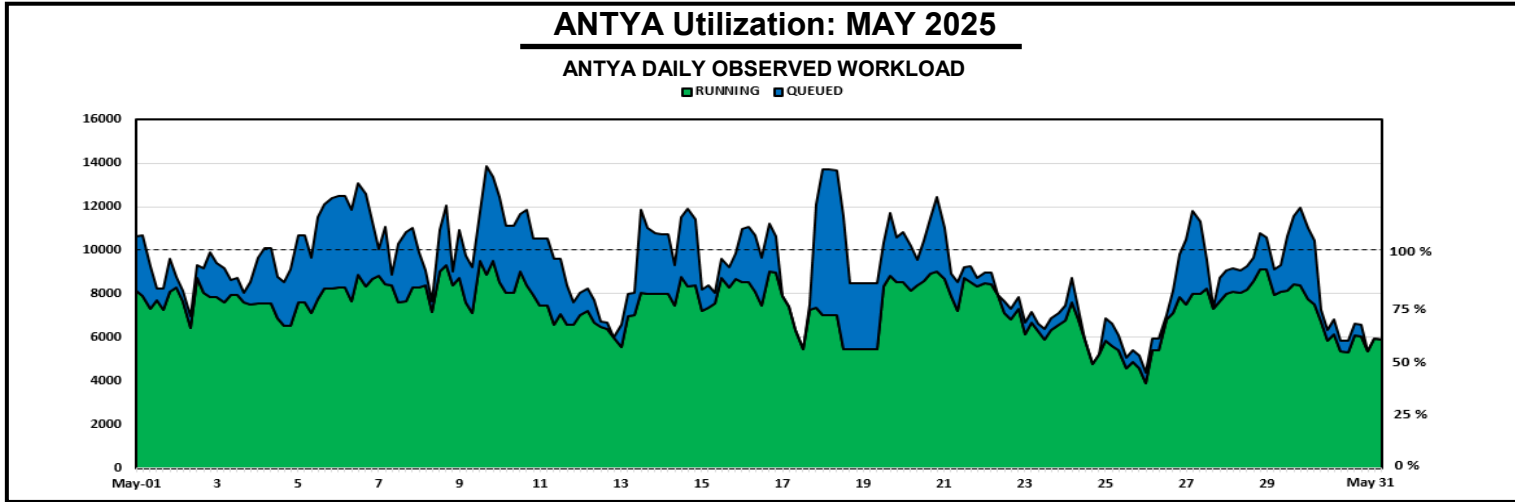
```
[user@cn234 ~] $ spack load lammps@20240829.1
```

```
[user@cn234 ~] $ mpirun -np 40 lmp -in in.nemd
```

```
## User may add above commands in PBS Batch script to submit job on compute nodes using spack
```

Spack gives user complete control over how software is built and configured in an HPC environment. Using LAMMPS as a case study in this article, we've seen how to:

- Customize software installations using variants
- Control compilers, dependencies, and hardware targets
- Use reproducible environments
- Avoid conflicts with system software



ANTYA HPC Users' Statistics

May 2025

Total Successful Jobs~ 1410

◆Top Users (Cumulative Resources)

CPU Cores

Amit Singh

Walltime

Amit Singh

Jobs

Jugal Chowdhury

ANTYA Usage, Updates and News

• **Scheduled Downtime:** There was no downtime of ANTYA for May 2025.

• **Job Submissions:** The highest job loads were observed in the *regularq*, *serialq*, *mediumq*, and *longq* queues, reflecting sustained user activity across multiple workloads in various queues.

• **Cluster Utilization:** The system maintained an average utilization of approximately 74.39% and peak utilisation of 95.08%.

Packages/Applications Installed: Flexible Atomic Code (FAC) module has been installed on ANTYA.
\$ module load fac-latest

Other Recent Work on HPC

Intense laser interaction with an inhomogeneous plasma: Validation of electromagnetic fields and absorption at different polarization	Shakti Kushwaha
Simulation and Analysis of Electron Cyclotron Resonance Heating (ECRH) Scenarios for ADITYA-U Tokamak	Komal
Relativistic cylindrical and spherical plasma waves	Ardhendu Sekhar Mishra
Vlasov-Maxwell simulation of coherent electromagnetic wave and its kinetic instability in a hot magnetized plasma	Pooja
Understanding toroidal flow reversal in inboard limited Aditya-U plasmas using EMC3-Eirene simulations	Arzoo Malwal
Ion Temperature Effects on 3D ELM Blob Dynamics in the Tokamak	Souvik Mondal
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The Development of Nb3Sn CICC-based coil	Piyush Raj
Mode Interaction Induced Thermal Relaxations in a 1D Dusty Plasma	Ankit Dhaka

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