

SStack: Software Stacks for easier and cleaner software builds on HPC

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Objectives

- SOFTWARE HIERARCHY,
ENVIRONMENT MODULES AND
PACKAGE MANAGERS
- SSTACK

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Software hierarchy, environment modules and package managers

- **Software Hierarchy** organizes software into different layers.
- **Environment Modules** software tool that help manage user environments and dynamically modify environment variables.
- **Package managers** tools automate parts of software build process and enable ease of installing multiple versions and configurations.

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```
ssh %#1 bash %#2 bash %#3 %#4
-----/software/modules/1.923/lssc0-linux/modulefiles-----
abyss/2.1.0 bowtie/1.2.2 dot hammer/3.1b2 megahit/1.1.3 ont-guppy-cpu/2.1.3-1 salmon/0.12.0-alpha structure/2.3.4
admixtue/1.3.0 bowtie2/2.3.3 entap/0.8.4-beta hmer/5.0.2 openmpi/1.6.5 sambamba/0.6.7 subread/1.5.3
afni/1.2.0 bowtie2/2.3.4.1 ersa/1.1.2 homer/4.10 metacompass/1.1 openmpi/2.0.2 samblaster/0.1.24 subread/1.6.0
albacore/2.3.1 bracken/2.1 evidence_modeler/1.1.1 htseq/0.10.0 mga/0.1 openmpi/3.1.1 samtools/1.5 subread/1.6.3
anacapa/2018-4-11 braker/2.1.2 exonerate/2.2.0 htlib/1.6 miniasm/0.2 orca/3.0.0 samtools/1.6 svtyper/0.6.1
anaconda2/4.5.12 breakdancer/1.4.5 falcon/2018.31.08 htlib/1.8 miniasm/0.3 orca/4.0.0.2 samtools/1.8 tensorflow-gpu/1.8-git
anaconda3/4.5.12 bseqc/10868e7 falcon/171211 htlib/1.9 minimap/2.2.2 pandoc/2.2.1 samtools/1.9 tensorflow-gpu/1.8.0
angsd/0.923 busseeker/2.1.5 falcon/default htstream/0.3.0 minimap2/2.7 partitionfinder/2.1.1 scallop/0.10.2 tensorflow-gpu/default
anvio/5.0 busco/3.0.2 fasta/36.3.8g htstream/0.3.1 minimap2/2.12 pasa/2.3.3 scythe/c27cd75 tensorflow-gpu/git+cuda3.0
arcs/1.0.4 bwa/0.7.16a fastq_screen/0.11.4 htstream/1.0.0 mirdeep2/2.0.0.8 pathoscope/2.0.6 seqtk/1.3 tensorflow3-gpu/1.10.1
arks/1.0.2 camoco/0.6.1 fastq_screen/0.13.0 idba/1.1.3 miso/0.5.4 pb-assembly/0.0.4 shapeit/v2.r904 tigmint/1.1.2
augustus/3.3.0 canu/1.6 fastx_toolkit/0.0.14 ima2p/1 mmarge/1.0 perl-ls/5.22.1 sickle/85e5117 tophat/2.1.1
augustus/3.3.2 canu/1.7 findfungi/0.23.3 isoseq3/0.7.2 mndo99/2013 pftools/2.3 skewer/0.2.2 transabys/2.0.1
awscli/1.14.9 canu/1.8 flash2/2.2.0 isoseq3/3.1.0 mndo99/2017 phylip/3.697 pip/9.0.1 slurm/17.02.6 transdecoder/5.0.2
bam_readcount/0.8.0 ccs/3.3.0 freebayes/1.1.0 jellyfish/2.2.7 module-info kallisto/0.43.1 module-inf smrtlink/5.1.0.26412 transdecoder/5.5.0
bamm/1.7.3 cdhit/4.6.8 fseq/1.85 kat/2.4.2 kentutils/302.0.0 multiqc/1.0 mothur/1.39.5 slurm/latest trinity/2.5.1
bamtools/2.4.2 cdna_cupcake/5.8 gat/1.3.4 kmer_mask/r2015 multiqc/1.6 multiqc/1.7 mummer/3.23 r/3.4.2 umap/0.3.7
bamtools/2.5.1 centifuge/1.0.3 gausian/16 gcc/8.2.0 king/2.1.8 kmc/3.1.0 multiqc/1.5 multiqc/1.7 mummer/3.23 racon/1.2.1 umitools/0.5.5
barracuda/0.7.107h clusterflow/0.5 cmake/3.12.3 gdb/8.2 kmcr/2.0.6-beta multiqc/1.6 multiqc/1.7 mummer/3.23 raddl/6c4c43f use.own
bayescan/2.1 cogent/3.5 colony/2.0.6.5 genemark_et/4.38 kraken2/2.0.6-beta multiqc/1.7 mummer/3.23 raddl/6c4c43f vcflib/7e3d806
bcftools/1.6 cogent/3.5 crossmap/0.3.1 genemark_et/4.38 kraken2/2.0.6-beta multiqc/1.7 mummer/3.23 raddl/6c4c43f vcftools/0.1.15
bcftools/1.8 csem/2.4 cutadapt/1.15 genrich/0.5 lastz/1.04 ldhelmet/1.10 lima/1.8.0 musc/3.8.31 randfold/2.0 recon/1.08 repeatmasker/4.0.7 vcontact/2.0.9.5
bcl2fastq/2.20.0.422 cutadapt/1.16 gffcompare/0.10.1 links/1.8.6 locuszoom/1.4 lumpy-sv/0.2.13 nanopolish/0.9.0 repeatscout/1.0.5 star/2.5.3a star/2.6.0c star/2.6.1d star/2.7.0e stringtie/1.3.3b stringtie/1.3.4d
bedops/2.4.30 cutadapt/2.0 gffread/0.9.9 macs2/2.1.1.20160309 macs2/2.1.2 maker/3.01.02-beta masurca/3.2.2 masurca/3.2.8 mcl/14-137 null salmon/0.9.1
bedops/2.4.33 cutadapt/2.0 gffread/0.9.12 gmap/2018-07-04 gmap/2018-07-04 gpflow/1.2.0 delly/0.7.2 delly/0.7.7 delly/0.7.8 diamond/0.8.31
bedtools2/2.26.0 cython/0.27.3 dbccomplicons/0.8.6 deepctools/2.5.4 gmap/2018-07-04 gpflow/1.2.0 delly/0.7.2 delly/0.7.7 delly/0.7.8 diamond/0.8.31
bedtools2/2.27.0 cython/0.27.3 dbccomplicons/0.8.6 deepctools/2.5.4 gmap/2018-07-04 gpflow/1.2.0 delly/0.7.2 delly/0.7.7 delly/0.7.8 diamond/0.8.31
bioperl/1.6.924 cython/0.27.3 dbccomplicons/0.8.6 deepctools/2.5.4 gmap/2018-07-04 gpflow/1.2.0 delly/0.7.2 delly/0.7.7 delly/0.7.8 diamond/0.8.31
bioperl/1.7.3 cython/0.27.3 dbccomplicons/0.8.6 deepctools/2.5.4 gmap/2018-07-04 gpflow/1.2.0 delly/0.7.2 delly/0.7.7 delly/0.7.8 diamond/0.8.31
biopython/1.71 cython/0.27.3 dbccomplicons/0.8.6 deepctools/2.5.4 gmap/2018-07-04 gpflow/1.2.0 delly/0.7.2 delly/0.7.7 delly/0.7.8 diamond/0.8.31
blast/2.2.31+ delly/0.7.2 delly/0.7.7 delly/0.7.8 diamond/0.8.31
blast/2.7.1+ delly/0.7.2 delly/0.7.7 delly/0.7.8 diamond/0.8.31
blast/2.8.1+ delly/0.7.2 delly/0.7.7 delly/0.7.8 diamond/0.8.31
blat/v.35 delly/0.7.2 delly/0.7.7 delly/0.7.8 diamond/0.8.31
boost/1.67 delly/0.7.2 delly/0.7.7 delly/0.7.8 diamond/0.8.31
-----/software/modules/modulefiles_static-----
annovar/2015-03-22 cellranger/2.0.1 clc/12.0 gatk/3.5 java/jdk1.8.0_05 picard-tools/1.91 rnammer/1.2 snpeff/4.3p trf/4.0.9
annovar/2018-04-16 cellranger/2.1.0 cluster_one/1.0 gatk/3.6 java32/jre1.8.0_60 picard-tools/1.114 rtg/3.6.2 snpeff/4.3t trim_galore/0.3.8
aspera-connect/3.5.1 cellranger/2.1.1 danpos/2.2.2 gatk/3.7 longranger/1.0.0 picard-tools/1.122 rtg/3.7.1 snver/0.5.3 trim_galore/0.4.3
bayestraits/2.0 cellranger/2.2.0 dmd/2.078.2 gatk/3.8 longranger/1.2.0 picard-tools/1.129 score-client/1.4.0 sspace/LongRead-1.1 trim_galore/0.4.5
bbmap/33.65_java7 cellranger/3.0.2 fastqc/0.11.2 gatk/4.0.5.2 longranger/2.1.5 picard-tools/1.139 segemehl/0.2.0 sspace/STANDARD-3.0 trim_galore/0.5.0
bbmap/36.86 checkm/1.0.7 fastqc/0.11.5 gcta/1.24.4 longranger/2.1.6 picard-tools/2.6.0 sicer/1.1 supernova/1.2.1 trim_galore/0.6.0
bbmap/37.68 clc/7.5 fastqc/0.11.7 hapcut/0.7 longranger/2.2.2 picard-tools/2.15.0 sifter/2.1.1 supernova/1.2.2 trimomatic/0.33
beagle/4.1 clc/7.5.5 gapfiller/1.10 interproscan/5.27-66.0 mash/2.0 picard-tools/2.18.4 signalp/4.1c supernova/2.0.0 trinotate/2.0.1
bismark/0.15.0 clc/8.0 gatk/3.1-1 interproscan/5.30-69.0 matlab/R2016a pilon/1.18 smrtanalysis/2.3.0-140936.p0 supernova/2.0.1 trinotate/3.0.0
bismark/0.17.0 clc/8.5.1 gatk/3.2-2 isode/1.0.0 metabat/2.12.1 platanus/1.2.1 snpeff/4.1i supernova/2.1.1 trinotate/3.0.1
bismark/0.19.0 clc/9.5 gatk/3.3-0 jalview/2.8.2 nsplice/0.9 qualimap/2.2.1 snpeff/4.1j targets/1.1 trinotate/3.1.1
bismark/0.20.0 clc/10.1 gatk/3.4-0 java/jdk1.7.0_75 pantherscore/1.03 rdptools/2.0.2 snpeff/4.3e tassal/3.0.171 virusfinder/2.0
bismark/0.20.1 clc/11.0.1 gatk/3.4-46 java/jdk1.8 pantherscore/2.1 refined-ibd/12Jul18 snpeff/4.3i tmhmm/2.0c weblogo/2.8
msettles@tadpole:/share/workshop/msettles/cli$
```

https://ucdavis-bioinformatics-training.github.io/2019_April_ESALQ_Microbial_Community_Analysis/cli/cluster.html



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SStack



- The Software Stack tool – manager of package managers.
 - Enables an easy way to install software with site-specific defaults.
 - Provides an option to represent all software on an HPC cluster in a hierarchical structure.

SStack terminology

- SStack - name of this tool.
- Stack - a single instance or installation of a stack type.
- Stack Type - specific package manager deployed in stack.
- Module - a lua file used by the Lmod Module System.
- Module Tree - a collection of modules.
- SStack Data Root or Path - top-level directory where SStack stores stacks, modules, and a stateful JSON.

SStack Structure

```
data_root (Default:~/sstack/osID_name)
├── modules
│   ├── stack_type
│   │   └── stack_name.lua
├── stacks
│   ├── stack_type
│   │   ├── stack_name
│   │   │   ├── stack_installation_data
│   │   │   └── ...
└── stacks.json
```

SStack Structure

```
~/sstack
├── centos7
│   ├── modules
│   │   └── spack
│   │       └── 2022a.lua
│   └── stacks
│       └── spack
│           └── 2022a
├── rhel8
│   └── modules
│       ├── custom
│       │   ├── 2022a.lua
│       │   ├── 2023a.lua
│       │   └── 2024a.lua
│       ├── spack
│       │   ├── 2022a.lua
│       │   └── 2023a.lua
│       ├── pixi
│       │   └── 2024a.lua
│       ├── sstack
│       │   └── main.lua
│       └── conda
│           ├── 2022a.lua
│           ├── 2023a.lua
│           └── 2024a.lua
```

```
└── stacks
    ├── custom
    │   ├── 2022a
    │   ├── 2023a
    │   └── 2024a
    │       ├── builds
    │       ├── modules
    │       ├── packages
    │       └── sources
    ├── spack
    │   ├── 2022a
    │   └── 2023a
    ├── pixi
    │   └── 2024a
    ├── sstack
    ├── conda
    │   ├── 2022a
    │   ├── 2023a
    │   └── 2024a
    └── stacks.json
```

SStack Installation

Dependencies:

- Lmod \geq 8.2.7
- curl, tar, bzip2, git, make
- writable and executable /tmp and \$HOME directories

```
# Install SStack (Install to default directory in ~/
sstack)
curl -fsSL "https://gitlab.com/nmsu_hpc/sstack/-/raw/main
/share/install_sstack_latest.sh"
| bash -s --

# Install to custom directory
curl -fsSL "https://gitlab.com/nmsu_hpc/sstack/-/raw/main
/share/install_sstack_latest.sh"
| bash -s -- "/software/sstack"

# Install to custom directory and set custom stack name
## This can be used to reinstall a broken sstack
installation
curl -fsSL "https://gitlab.com/nmsu_hpc/sstack/-/raw/main
/share/install_sstack_latest.sh"
| bash -s -- "/software/sstack" "latest-el7"
```



SStack Types



Custom

Installing Spack Stack

```
$ module use ~/sstack/modules
$ module load sstack
$ sstack install --name 2023a --type spack
...
Stack Successfully Installed!
+-----+-----+-----+-----+
| Name   | Type   | Version | Path                                     |
+-----+-----+-----+-----+
| 2023a  | spack  | 0.18.0  | ~/sstack/stacks/spack/2023a           |
+-----+-----+-----+-----+

$ module load spack/2023a
$ spack --version
0.18.0 (c09bf37ff690c29779a342670cf8a171ad1b9233)

$ spack install zlib
[+] /home/username/sstack/stacks/spack/2023a/opt/spack/
    linux-fedora35-x86_64_v3/gcc-11.3.1/zlib-1.2.12-
    ojxmrh7kuyqszihdl5573b4pjadftkld

$ module spider zlib
-----
zlib: zlib/1.2.12-ojxmrh7
-----

You will need to load all module(s) on any one of the
lines below before the "zlib/1.2.12-ojxmrh7" module
is available to load.

    spack/2023a

Help:
A free, general-purpose, legally unencumbered
lossless data-compression
library.
```



Module avail

```
$ module avail
```

```
----- /fs1/home/user/sstack/rhel_8/modules -----  
conda/2023b  pkgsrc/2024a  spack/2023b (D)  
  
----- /fs1/software/sstack/rhel_8/modules -----  
conda/2022a  conda/2023a  conda/2024a (D)  
custom/2022a custom/2023a  custom/2024a (D)  
pixi/2024a   spack/2022a  spack/2023a   sstack/main  
  
----- /etc/modulefiles -----  
pmix/2.2.5   pmix/3.2.3   pmix/4.1.2 (D)  
  
----- /fs1/software/sstack/modules -----  
os/centos_7_test (S)  os/centos_7 (S)  
os/rhel_8_test (S)  os/rhel_8 (S,L,D)  
  
----- /usr/share/lmod/lmod/modulefiles/Core -----  
lmod  settarg
```



Searching for module

```
$ module spider python
```

```
python:
```

```
Versions:
```

```
python/3.9.12-2022a-gcc_12.1.0-x3yusmt  
python/3.9.12-2022a-gcc_12.1.0-ys2veed  
python/3.10.8-2023a-gcc_7.5.0-enoj4ib  
python/3.10.8-2023a-gcc_12.2.0-hvrnktz
```

```
For detailed information about a specific "python"  
package (including how to load the modules) use the  
module's full name.  
Note that names that have a trailing (E) are extensions  
provided by other modules.  
For example:
```

```
$ module spider python/3.10.8-2023a-gcc_12.2.0-  
hvrnktz
```

Searching for module

```
$ module spider python/3.10.8-2023a-gcc_12.2.0-hvrnktz
```

```
-----  
python: python/3.10.8-2023a-gcc_12.2.0-hvrnktz  
-----
```

You will need to load all module(s) on any one of the lines below before the "python/3.10.8-2023a-gcc_12.2.0-hvrnktz" module is available to load.

```
spack/2023a gcc/12.2.0-2023a-gcc_8.5.0-e643dqu
```

Help:

The Python programming language.



Thank you!

https://gitlab.com/nmsu_hpc/sstack

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