

Builtin software

The OAsis HPC cluster has some standard software built-in. We provide them via Lmod and Containers. Users may choose the way they are comfortable with.

Lmod

All software and module files are put in the parallel file system, and accessible in any compute nodes and login nodes. To compile your code, you may load a specific MPI toolchain in a login node. And use the same MPI version to run your program on compute nodes.

We provide various versions for each software. To prevent loading incompatible sets of modules, our Lmod uses [a software hierarchy](#). For example, to load FFTW 3.3.10 using the OpenMPI 4.1.4 plus GCC 11.3 toolchain, you may execute the following statement:

```
module load GCC/11.3.0 OpenMPI/4.1.4 FFTW.MPI/3.3.10
```

Later, when you want to load, e.g., the BLAST module. You don't have to worry about the incompatible toolchain because of the help from the module system.

Browse modules on the web portal

Log in to the web portal, click Supports, then Software, and you will see a graphical module browser. You may search for any keyword, check available versions, and copy the loading statement.

Browse in console

To browse the catalog in log in node, use the standard Lmod spider command:

```
# see the full catalog for all available module
module spider

# search with keyword
module spider openmpi

# search for the document of a specific version
module spider openmpi/4.1.4
```

To browse modules supported by a toolchain:

```
module load GCC/11.3.0
module avail
```

If you are interested in the details, please check out the [Lmod documentation](#).

Containers

Another way to run software on the cluster is to use containers, which is another good way to avoid library incompatibility. Since all libraries are built into a portable container image, we don't need to load any module in advance.

Most of our examples use containers. Also, software in containers is often more up-to-date.

The cluster-provided containers are located at `/pfss/containers`. This folder is shared by all login nodes and compute nodes. In addition, we provide several GPU and MPI-ready containers for you to kick-start your workload.

Similar to Lmod, we have a polished browser on our web portal. Head to supports, software, then containers. Besides the provided containers, you should also see your containers there. The browser looks for any containers placed in the containers folder in any of your file sets. For example, `/pfss/home/loki/containers` and `/pfss/scratch02/oneasia` for the user loki of group oneasia.

Revision #15

Created 4 November 2022 07:42:13 by Loki Ng

Updated 13 November 2022 17:08:37 by Loki Ng