Accessing Software

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Overview

The policies regarding the installation of software are on this page. In general, scientific software is installed as requested with the caveats noted in that section. There are over 100 software applications installed as modules. You should look there first. And you are always welcome to install your own software or other software in your file space.

CentOS 6 and CentOS 7

Puma is built with CentOS 7 along with the system libraries, compilers and utilities that are needed for HPC operations.

Ocelote is built with CentOS 6 along with the relevant system libraries, compilers and utilities. Some workloads need CentOS 7 for its newer kernel. A number of GPU nodes have been reprovisioned with a CentOS 7 image. To access one of these nodes, modify the PBS select statement to include 

```
select=1:ncpus=28:mem=224gb:np100s=1:os7=True
```

More information is here

Elgato is also built on CentOS, and is kept consistent with Ocelote. The big difference is that Elgato does not have a comprehensive suite of software, by design.

Installed software

A list of installed software is kept at this page, but may not be as current as using the `module avail` command as shown below.

Modules

Many popular software packages are installed and available as modules. There may be several versions of a package available.

<table>
<thead>
<tr>
<th>Module Command</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>module avail</td>
<td>Display all the software and versions installed on the system</td>
</tr>
<tr>
<td>module avail gromacs</td>
<td>Display all installed versions of Gromacs</td>
</tr>
<tr>
<td>module list</td>
<td>Display the software you have loaded in your environment</td>
</tr>
<tr>
<td>module what-is .modulename</td>
<td>Displays some descriptive information</td>
</tr>
</tbody>
</table>
Installing additional software

To submit a request to have software installed on the UA HPC systems use the HPC Software Install Request form: https://it.arizona.edu/hpc-software-install-request

There is no expected timeframe for how long it takes to install software. There are many variables. If you haven't heard back in a week, it is reasonable for you to follow up with hpc-consult@list.arizona.edu

You can install software packages into your home directories with the space that is allocated to you with your HPC account. However you cannot install software that requires root permission, or use a method like "yum install" that accesses system paths.

Follow this link for detailed information on how to install your own software

Using Perl

Follow this link for more information on using Perl.

Using Python

Follow this link for more information on using Python.

Using R

Follow this link for more information on using R.

Using Matlab

Follow this link for more information on using Matlab

Using Anaconda

Anaconda is available as a module and comes with Glueviz, JupyterLab, Jupyter Notebook, Spyder, Orange and RStudio. It also supports the conda commands for building a personal environment.

More details are at this page.

Using Spark

Apache Spark is a fast and general-purpose cluster computing system. However it has not been installed for support in a multi-node environment as yet. That functionality is planned for the future. It provides high-level APIs in Java, Scala, Python and R, and an optimized engine that supports general execution graphs. It also supports a rich set of higher-level tools including Spark SQL for SQL and structured data processing, MLlib for machine learning, GraphX for graph processing, and Spark Streaming.

There are some simple tests here.

Compilers

- El Gato
  - El Gato is now running CentOS 7. The compilers available are:
    - Intel/2019.3: "module load intel"
    - GCC 5.4.0: "module load gnu"
    - GCC 8.3.0: "module load gnu8"
    - LLVM 5.0.1: "module load llvm5"

- Ocelote
  - GCC is available without loading a module. gcc --version shows that it is 6.1.0. If you also need the GNU Scientific Libraries (gsl), that is available using module load gsl which will get you version 2.1
  - The Intel Compiler suite 2016 is available in both 32 and 64 bit versions. The math kernel libraries (mkl) are provided as separate modules, also in 32 and 64 bit versions.
The Intel Compiler 2019 is available and is no longer separated like 2016. So there are not separate modules for mkl, mpi, etc.

PGI compilers 2018 (Portland Group) are installed as a module. We have provided these in particular for their OpenACC support. We do not build software with the PGI compilers.

MPI. There are more choices now so pay attention.
- There are standard Red Hat versions of mpich, mvapich, mvapich2 and openmpi. Some extra options are invoked when you load one - use `module avail` to see the specific name.
- The same four MPI are available with more detailed options for gcc, intel and open64. Again use `module avail` for the appropriate choices.

AVX2 Ocelote has Intel V3 Haswell processors. A key feature of these is AVX2. Read this Intel document.

For AVX2 support, compile with the `-xHOST` option. Note that `-xHOST` alone does not enable aggressive optimization, so compilation with `-O3` is also suggested. The `-fast` flag invokes `-xHOST`, but should be avoided since it also turns on interprocedural optimization (`-ipo`), which may cause problems in some instances.

For GNU compilers, AVX support is only available in version 4.6 or later. For AVX support, compile with `-mavx`