Environment Modules

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Environment modules are used to provide the dynamic modification of a user's environment via modulefiles.

Easy way to alter or change environment variables such as $PATH or $LD_LIBRARY_LOAD.

Be careful not to confuse "environment modules" with "kernel modules."

Using modules

module avail
shows the available modules in $MODULEPATH. Long output with `-l`

module add|load *Modulename*
load the module with the modulename (output from module avail).
Possible to load multiple modules.
Modules not in $MODULEPATH can be loaded with the full or relative path. (But not only filename!)

Using modules

rm|unload *Modulename*
unload the module

module purge
unload all modules

module list
list all loaded modules

module show *Modulename*
Display information about one or more modulefiles

Using modules

module use *Directory*
Add *Directory* to the first position of $MODULEPATH. To append use `-a`.

module unuse *Directory*
Remove *Directory* from $MODULEPATH

Using modules
Examples

```
[sblock@frontend01 ~] module avail -l
- Package -----------------+- Versions -+- Last mod. -----

/cluster/modulefiles:
comp/gcc/7.2.0                           2017/12/30 16:39:34
julia/0.6.2                              2018/06/06 11:24:58
mpi/openmpi/gcc/3.0.0                    2017/12/30 17:16:45
mpi/openmpi/gcc/3.1.2                    2018/10/09 12:31:01
mpi/openmpi-java/gcc/3.0.0               2018/06/05 14:35:26
mpi/openmpi-x86_64                       2017/08/03 20:28:39
nvidia/cuda/9.0                          2018/02/07 13:41:18
nvidia/cuda/9.2.88                       2018/05/31  8:50:48
singularity/2.5.2                        2018/10/12 12:48:52
```

Using modules
Examples

```
module load mpi/openmpi/gcc/3.1.2 comp/gcc/7.2.0
module list
Currently Loaded Modulefiles:
 1) mpi/openmpi/gcc/3.1.2   2) comp/gcc/7.2.0
module purge
module load /home/users/s/sblock/modules/turbomole_test
module list
Currently Loaded Modulefiles:
 1) turbomole_test
```

Using modules

module load can be included in the shell's initialization file (.bash_profile, .bashrc, ...) or in sbatch scripts.
It can be used in bash scripts but then it is only available in the scripts sub-shell.

After loading a module on fronted the environment is used when running srun, salloc or sbatch.

```
[sblock@frontend01 ~]$
srun gcc --version
  gcc (GCC) 4.8.5 20150623 (Red Hat 4.8.5-16)
module load comp/gcc/7.2.0
srun gcc --version
  gcc (GCC) 7.2.0
```

Using modules

module is a function and can not used with srun.

```
srun module list
```

will fail!

To load a module from your current directory use ./modulname.

```
module load ./modulename
```

module can load environment including aliases and other modulefiles. If someone is interested in writing own module files I can prepare a presentation.

Cluster news

- Fairshare works different now. The calculation is still based on used resources. However this is no longer reset every month but calculated with a decay half life time of 7 days.
- The base amount of fairshare shares was changed to respect the higher priority for accounts/users belonging to eecs (Faculty IV).
- The priority weight was changed in some ways:
  PriorityWeightAge = 4000
  PriorityWeightFairShare = 20000
  PriorityWeightJobSize = 1000
  PriorityWeightPartition = 30000

Cluster news

- OpenMPI 3.1.2 is now available on the cluster. It can be used with the modulefile `mpi/openmpi/gcc/3.1.2`
- The containerization program Singularity version 2.5.2 is now available and loadable with the modulefile `singularity/2.5.2`
- The OmniPath hardware on SMP001 was replaced.
- The NUMA (Non-uniform memory access) configuration is now set correct on node070 and node132

Using sshfs

An easy way to access the files on the cluster storage is *sshfs*. This way you can mount remote directories over ssh.

1. create a local mount point
   ```
   mkdir ~/clustermnt
   ```
2. mount the remote folder:
   ```
   sshfs user@gateway.hpc.tu-berlin.de:  ~/clustermnt/
   ```
3. the user cluster home folder is now mounted to ~/clustermnt/
4. To unmount close all open files in ~/clustermnt and leave the directory in the shell or your file manager. Then umount:
   ```
   fusermount -u ~/clustermnt
   ```

Notes about sshfs

The remote folder to mount can be relative to home with `:directory` or the absolute path `:/path/to/directory`.

Editing or creating files inside the sshfs-mount is done as user (on the cluster), not the local user.

sshfs is easy but not fast.

correction of the last presentation

The nodes gpu[001-020] have **512GB** of memory, not 256GB.

gpu21 also has two Nvidia Tesla but only 256GB of memory.