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Atomic simulation for energy solutions

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Set up Environmental Module in a CentOS6 + Rocks system

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Module is a convenient way to manage shell environment variables and aliases. And it is simple enough for linux novice users to use the right software/compiler that they want. As far as I know, there are two module software, lmod and environmental module using tcl language. Our cluster OS came with Environmental Module 3.2.10.

1. Customize module path (only needed for adding a new parent folder for modulefiles)

the Module software searches in an environment variable, **MODULEPATH**, for available modulefiles. The first step is to add a new folder to this environment variable **MODULEPATH** and thus we can put all the customized-modulefile in this new folder. I don't want to revise the system default module folder, like `/usr/share/Modules/modulefiles` and `/etc/modulefiles`, so that we can also distinguish our adaption to the system default modules.

```
mkdir -p /share/apps/Modules/modulefiles echo "  
export MODULEPATH=${MODULEPATH}:/share/apps/Modules  
/modulefiles" >>/etc/profile.d/modules.sh
```

Since the files in `/etc/profile.d` are not automatically sync to compute nodes. We can push this change manually. The *for* loop will loop over all nodes and copy the `.sh` file from the master node to the compute node.

```
rocks run host compute command="echo "export  
MODULEPATH=${MODULEPATH}:/share/apps/Modules/modulefiles" >>/etc  
/profile.d/modules.sh"
```

However, this is not enough. This manual push will be purged if the compute node is reinstalled. (for example, rocks will reinstall the compute node after a power outage, not reboot though.)

We also need to add this change into the distro. See **official manual here**.

```
vi /export/rocks/install/site-profiles/6.1/nodes
```

#edit the file and add a line in the post installation section.

```
<post> ...
```

```
echo "export MODULEPATH=\$MODULEPATH:/share/apps/Modules/modulefiles" >>/etc/profile.d/modules.sh
```

```
</post>
```

Rebuild the distribution

```
cd /export/rocks/install rocks create distro
```

We don't need to do anything for the /share/apps/Modules folder, since /share/apps are automatically updated to all compute nodes.

2. Add in module files

The module file has to be written in TCL and put in the folder /share/apps/Modules

At the moment, I only add several files for vasp and mpi. I learn the format by official manual of module, modulefile and

```
module show null module show modules
```

and the example on XSEDE machines.

Here's a list of the new module added.

```
mpich: 3.0.3 openmpi: 1.6.4 vasp: 5.4.1-mpich 5.4.1-openmpi-1.6.4
```

3. set up the default version

add a ".version" file at the module folder you want like below

```
cd /share/apps/Modules/mpich-3.0.3/qe
cat > .version <<EOF
#%Module1.0
set ModulesVersion "6.0"
EOF
```

See also: **System Administration**