MAPS

Category
Chemistry, Commercial, Visualization

Description
MAPS is a front-end to various Computational Chemistry software, including lammps, Quantum ESPRESSO and ABINIT.

Version
4.0

Official Website
http://www.s16080558.onlinehome-server.info/

Licensing Terms and Conditions
MAPS is a commercial software. Unauthorized usage is strictly forbidden.

Simulation as Batch Job on Dalma

Once you have your case directory ready (e.g., the directory where run.py resides), you can submit a job on Dalma to do the computation. Follow the steps below.

1. Upload or prepare your case directory to Dalma, preferably on $SCRATCH.
2. Login Dalma. Within the terminal, go the case directory. When you run ls, you should see something like this.

   [gh50@login-0-1 waterbox_nvt]$ ls
   runinfo run.py waterbox_nvt.data
   waterbox_nvt.in waterbox_nvt.py

3. (Optional) In file runinfo, you can change the number of processes to use for your job. E.g.,

   [gh50@login-0-1 waterbox_nvt]$ cat runinfo
   # log for run.py
   info : remove GPU keywords
   executable : lammps
   command : mpirun -np 56 lammps -in
   "waterbox_nvt.in" -log "waterbox_nvt.log" -screen
   "waterbox_nvt.err"

   You can change 56 to a different number that can be divided by 28 (e.g., 56, 84, 112, ...).
4. Run the following commands to generate a job script called dalma-slurm-maps-job.sh in the same folder.
module load maps
give-me-maps-jobs.sh

Example:

[gh50@login-0-1 waterbox_nvt]$ module load maps
Loading module 'maps/4.0'
[gh50@login-0-1 waterbox_nvt]$ give-me-maps-jobs.sh
dalma-slurm-maps-job.sh generated.

5. (Optional) The default walltime is 30 minutes. You could change it by modifying this line.

```bash
#SBATCH --time=00:30:00
```

6. Now you can submit the job.

```bash
sbatch dalma-slurm-maps-job.sh
```

**FAQ**

- Can I run multiple jobs under one case directory?
  No, you can only run one job under one case directory.
- Can I run VASP with MAPS on Dalma?
  No, you need to buy extra license for VASP.