NSF/IUCRC CAC PROJECT

INTEGRATED VISUALIZING, MONITORING, AND MANAGING HPC SYSTEMS

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JOB INFORMATION


```
"1934015": {
        "cpu_cores": 36,
        "finish_time": 1597383300000000000,
        "job_name": "RASPA_H2S",
        "node_list": [
          "10.101.7.57-36"
        ],
        "start_time": 1597210090000000000,
        "submit_time": 1597210055000000000,
        "total_nodes": 1,
        "user_name": "ipandey"
    }
```

MORE JOB INFORMATION

- More info about a job
  - Modules the job is using
  - What kind of problems the job is solving
  - …
- Getting job scripts (based on UGE)
  - Running job scripts can be found in the **UGE spool directory**, e.g. /export/uge/default/spool/compute-9-41/compute-9-41/job_scripts/1931693
  - Finished job scripts may be found in the **Lustre file system**, e.g. /lustre/scratch/zhu40264/Tian/Black_Marble/COLD-master/AsubmitJob_smp_mon.sh, if the user does not remove the script file

Ref: https://discl.cs.ttu.edu/gitlab/Misha.Ahmadian/HPC_Provenance

JOB SCRIPTS EXAMPLE

```
#!/bin/bash

#$ -V

#$ -cwd

#$ -j y

#$ -S /bin/bash

#$ -N Visc_340

#$ -o $JOB_NAME.o$JOB_ID

#$ -e $JOB_NAME.e$JOB_ID

#$ -P quanah

#$ -q omni

#$ -pe mpi 144


module load intel impi lammps netcdf python2

mpirun --machinefile machinefile.$JOB_ID -np $NSLOTS lmp_mpi -in
input.nemd
```

Lammps: a classical molecular dynamics simulation code with a focus on **materials modeling**.

Netcdf: a set of libraries and data formats that support creation, access, and sharing of **array-oriented** scientific data.

Ref: https://lammps.sandia.gov/doc/Manual.html, https://www.unidata.ucar.edu/software/netcdf/docs/index.html

QUESTIONS?/COMMENTS?