

# NAMD

**Purpose:** Molecular Dynamics

**Latest version:** 2.13

**License:**  Free of use for non-commercial users

*Mixed license \_ext-link*

**Website:** *http://www.ks.uiuc.edu/\_ext-link*

**NAMD** is a molecular dynamics package.

NAMD implements standard MD capabilities (variety of integrators, thermostats, barostats, force field compatibility, PME electrostatics, time-step integration, replica exchange, free energy calculations, etc.).

NAMD is also available to run on GPU NODES showing up to 8X performance (at same number of cores as std nodes). To perform GPU computations, please *contact us*.

## SLURM Submit script example

---

More information about the submit script can be found using the *Job Script Generator*.

### Sbatch options:

The options shown in the example are detailed below. For more information and a more comprehensive list of available options, see the *sbatch command page*.

- **-J:** Name for the job's allocation.
- **-e:** Name of the *stderr* redirection filename.
- **-o:** Name of the *stdout* redirection filename.
- **-p:** Name of the partition (queue) where the job will be submitted.

#### namd\_example.slm

```
#!/bin/bash
#SBATCH -J namd_example
#SBATCH -e namd_example.%j.err
#SBATCH -o namd_example.%j.out
#SBATCH -p std
#SBATCH -n 4
#SBATCH -t 02-00:00

module load apps/namd/2.13

##
# Modify the input and output files!
INPUT_FILE=namd_example.com
OUTPUT_FILE=namd_example.log

cp -r ${SLURM_SUBMIT_DIR}/${INPUT_FILE}
${SCRATCH}
cd ${SCRATCH}

srun `which namd2` ${INPUT_FILE} > ${OUTPUT_FILE}

cp ./${OUTPUT_FILE} ${SLURM_SUBMIT_DIR}
```

- **-n**: Number of tasks.
- **-t**: Set the job's time limit. If the job don't finish before the time runs out, it will be killed.

## Benchmarks

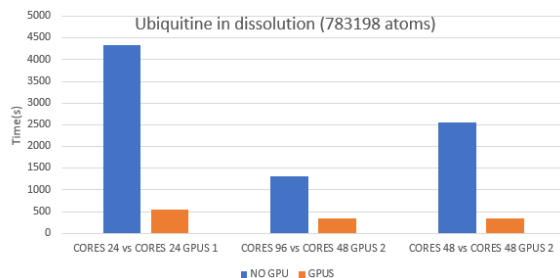


Fig: Comparison between jobs with and without GPGPUs.