NWChem

High-Performance Computational Chemistry

Introduction

NWChem aims to provide its users with computational chemistry tools that are scalable both in their ability to treat large scientific computational chemistry problems efficiently, and in their use of available parallel computing resources from high-performance parallel supercomputers to conventional workstation clusters.

Homepage

Installed versions

The following versions are currently installed :

- 6.1.1, not recommended, problems have been observed with this version
- 6.3-rev2-patch1, current release with QMD patch applied. Compiled with Intel compilers, MKL and Intel MPI
- 6.3-rev2-patch1-openmpi, same as above, but compiled with OpenMPI and NWChem provided BLAS instead of MKL. This version is expected to be slower
- 6.3-rev2-patch1-venus, this version contains only libraries for VENUS interface linking. Does not provide standalone NWChem executable

For a current list of installed versions, execute :

```
module avail nwchem
```

Running

NWChem is compiled for parallel MPI execution. Normal procedure for MPI jobs applies. Sample jobscript :

```
#PBS -A IT4I-0-0
#PBS -q qprod
#PBS -l select=1:ncpus=16

module add nwchem/6.3-rev2-patch1
mpirun -np 16 nwchem h2o.nw
```

Options

Please refer to the documentation and in the input file set the following directives :

- MEMORY : controls the amount of memory NWChem will use
- SCRATCH_DIR : set this to a directory in SCRATCH filesystem (or run the calculation completely in a scratch directory). For certain calculations, it might be advisable to reduce I/O by forcing "direct" mode, eg. "scf direct"