GULP - General Utility Lattice Program

Scientific details about GULP can be found in the following papers:

1. GULP - a computer program for the symmetry adapted simulation of solids, J.D. Gale, JCS Faraday Trans., 93, 629 (1997)

License and Usage

GULP is available free of charge to academics provided you accept the following conditions of use: The program is not to be distributed to anyone else without the express permission of the author. The program is not to be used for commercial research. For any commercial use of the program a license must be obtained from Accelrys Inc, including contract research. The program is supplied on an "as is" basis with no implied guarantee or support.

To use GULP you must register via the Web site http://projects.ivec.org/gulp/. The registration process checks that your email address is from a valid educational institution domain. Examples include .edu, .edu.au, and .ac.uk. If your institution is not recognised by the system then email us - do not try to fool it. If your institution does not have students, then you must use the commercial version from Accelrys.

For commercial and government use, you must contact Accelrys Inc.

Running GULP on Invicta and Napier

GULP v4.0 has been compiled using the default environment. An environment module has been created which can be invoked as follows.

> module load gulp/4.0

> module list
Currently Loaded Modulefiles:
   1) openmpi/1.4.3/intel   2) intel/mkl/10.2   3) gulp/4.0
A sample job script for GULP on Invicta might look as follows, change to "ptile=24" for Napier.

```bash
#BSUB -J GULP
#BSUB -o stdout.%J.txt
#BSUB -e stderr.%J.txt
#BSUB -R "span[ptile=24]"
#BSUB -n 32
#BSUB -W 0:20

cd $LS_SUBCWD

# load modules
source /etc/profile.d/modules.sh
module load gulp/4.0

export myexe="gulp"
export myargs="< inputfile > outputfile"

# count how many processors are allocated
NP=0
for TOKEN in $LSB_HOSTS
do
    ((NP++))
done

# now run GULP
mpiexec.hydra -np $NP $myexe $myargs

This can be submitted to the LSF queue using the bsub command.

Further Information

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