SIESTA

Sieta: Electronic Structure and Molecular Dynamics

Introduction

SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) is both a method and its computer program implementation, to perform electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids.

Please consult the Siesta Home page for further details and documentation.

Licensing and Versions

Leibniz Computing Centre makes use of the academic license for this package. Please note that you are required to obey the license restrictions as laid out on the SIESTA web site. Please consult these web pages before using SIESTA on the LRZ HPC systems.

The command "module avail siesta" gives information about the available versions, and also which version will be loaded by default.

Usage

It is normally necessary to use SIESTA in batch mode; for this purpose example job scripts are provided below, which of course need modification for specific usage. Prior to invoking the program, the environment module siesta must be loaded.

```
#!/bin/bash
#SBATCH -o /home/cluster/<group>/<user>/mydir/vasp.%j.out
#SBATCH -D /home/cluster/<group>/<user>/mydir
#SBATCH -J <job_name>
#SBATCH -M mpp1
# or use icel for the agi ICE etc.
#SBATCH --ntasks=32
#SBATCH --mail-type=end
#SBATCH --mail-user=<email_address>@<domain>
#SBATCH --export=NONE
#SBATCH --get-user-env
#SBATCH --time=24:00:00
#SBATCH --no-requeue
#SBATCH --account=insert your_projectID_here
#SBATCH --partition=insert test, micro, general, large or fat
.cd mydir
module load siesta
srun_ps $(which siesta)
```

```
#!/bin/bash
# Job Name and Files (also --job-name)
#SBATCH --jobname
#Output and error (also --output, --error):
#SBATCH -o ./%x.%j.out
#SBATCH -e ./%x.%j.err
#Initial working directory (also --chdir):
#SBATCH -D ./
#Notification and type
#SBATCH --mail-type=END
#SBATCH --mail-user=insert_your_email_here
# Wall clock limit:
#SBATCH --time=24:00:00
#SBATCH --no-requeue
#Setup of execution environment
#SBATCH --export=NONE
#SBATCH --get-user-env
#SBATCH --account=insert your_projectID_here
#SBATCH --partition=insert test, micro, general, large or fat
.cd mydir
export OMP_NUM_THREADS=1
module load siesta
mpirun --n 64 $(which siesta)
```

Documentation

Is available on the systems in PDF format. Please inspect the $SIESTA_DOC directory after loading the siesta environment module.
Support

Please contact the LRZ HPC support group if you experience any problems with SIESTA or have any questions on the usage of this application.