Phana on HPC

What is Phana?

PHonon ANAlyzer for Fix-Phonon (PHANFF) is a software tool for analyzing phonon properties in crystalline materials. It uses density functional perturbation theory (DFPT) to calculate phonon frequencies, phonon eigenvectors, and thermal properties such as heat capacity and thermal conductivity. PHANFF can also be used to perform phonon-phonon interaction calculations and to generate input files for other phonon-related simulations, such as Raman scattering or inelastic neutron scattering. The PHANFF package is an open-source software, written in FORTRAN and based on the Quantum ESPRESSO package.

Links:

Official Website

Versions Available:

The following versions are available on the cluster:

- phana- v2.75

How to load Phana?

To load Phana, use the following commands:

```
#Load the PHANA module
module load physical/phana/2.75
```

To verify if the module is loaded correctly, use the following command,

```
# List all the module loaded in the environment
module list
```

In a fresh environment, this should show only Phana since it is an independent software.

How to use PHANA?

To run the help section of phana use,

```
#Help section | see command line args
phana -h
```

Here is a sample slurm script to run phana,

```
#!/bin/bash
#SBATCH --job-name=phana_job
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=16
#SBATCH --time=24:00:00
#SBATCH --partition=normal
#SBATCH --output=phana_job.out
#SBATCH --error=phana_job.err
 #SBATCH -p main
#SBATHC --qos main
module load phana/version

# Prepare input file
phana_input_file="input.dat"

# Run PHANFF
phana < $phana_input_file > phana.out
```

Where to find help?

If you are confused or need help at any point, please contact OIT at the following address.

https://ua-app01.ua.edu/researchComputingPortal/public/oitHelp