LITESOPH INSTALL GUIDE

Prerequisites:

- Linux System (Ubuntu recommended)
- Miniconda
- Litesoph Dependencies

Step 1 - First install miniconda

open the terminal start by typing these commands to install miniconda

mkdir -p ~/miniconda3

wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh -O ~/miniconda3/miniconda.sh

bash ~/miniconda3/miniconda.sh -b -u -p ~/miniconda3

~/miniconda3/bin/conda init bash

Or you can refer this link if you want to know how to install
https://docs.conda.io/projects/miniconda/en/latest/index.html#quick-command-line-install

Step 1.1 - Create a conda environment

conda create -n myenv

conda create -n litesoph -- I have named this as my environment

conda activate litesoph -- to activate the environment

STEP 2 – Install Software Dependencies

1- NWCHEM
2- GPAW
3- Octopus

GPAW and NWCHEM

To install GPAW and NWChem in the same conda environment

conda install -c conda-forge gpaw nwchem python=3.10

OCTOPUS INSTALL

To install octopus you need to install spack first so do these steps

git clone -c feature.manyFiles=true https://github.com/spack/spack.git

source spack/share/spack/setup-env.sh

Note - You need to have a gcc and gfrotran compilers so check versions

gcc - - version
gfortran - -version

spack install octopus

Your compilers file should look like this

```
(litesoph) ashish@ashish:~$ cat /home/ashish/.spack/linux/compilers.yaml
compilers:
- compiler:
    spec: gcc@=11.4.0
    paths:
      cc: /usr/bin/gcc
      cxx: /usr/bin/g++
      f77: null
      fc: null
    flags: {}
    operating_system: ubuntu22.04
    target: x86_64
    modules: []
    environment: {}
    extra_rpaths: []
```

STEP 3 - LITESOPH

You can get the source code from the following command

- git clone -b main https://github.com/aitgcodes/litesoph.git
- cd litesoph
- pip install .

To edit the file

To create lsconfig file: litesoph config -c

To edit lsconfig file: litesoph config -e

STEP 3.1 - How to use the software

use command

- litesoph gui