

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

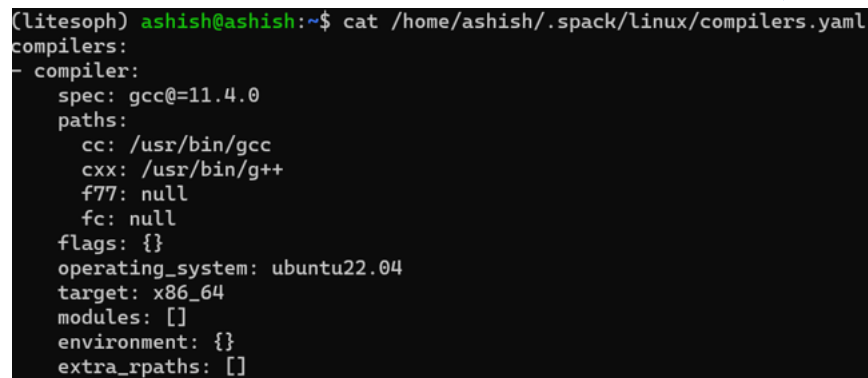
```
git clone -c feature.manyFiles=true https://github.com/spack/spack.git
source spack/share/spack/setup-env.sh
```

Note - You need to have a gcc and gfortran 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** Isconfig file: litesoph config -c

To **edit** Isconfig file: litesoph config -e

STEP 3.1 - How to use the software

use command

- litesoph gui

