Installation manual

1. Setting up the conda environment
   - Download miniconda package from https://repo.anaconda.com/miniconda/.
   - In linux terminal use the following comand
     - bash <filename>
   - In a new terminal then use the following commands to create environment,
     - conda create -n <environment name>
     - conda activate <environment name>
   - To install GPAW and NWChem in the same conda environment
     - conda install -c conda-forge gpaw nwchem python=3.10

2. OCTOPUS installation (on PARAM ANANTA):
   - First clone spack
     git clone -c feature.manyFiles=true https://github.com/spack/spack.git
   - Source spack for your shell,
     . spack/share/spack/setup-env.sh
   - copy compilers from another (already installed) spack to your spack package,
     cp /home/apps/spack/etc/spack/compilers.yaml /<path-to-your-spack>/spack/etc/spack/
     mkdir /home/msccp22/.spack
     spack config edit upstreams
   - To register the other Spack instance, you can add it as an entry to upstreams.yaml

     ```
     upstreams:
       spack-instance-1:
         install_tree: /path/to/other/spack/opt/spack
     ```

   - Now, to install **octopus-code**, use
     - Spack install octopus%oneapi

3. Litesoph installation
   - You can get the source code from the following command
     - git clone -b main https://github.com/aitgcodes/litesoph.git
     - cd litesoph
     - pip install .
4. Configuration
   - To create lsconfig file:
     - litesoph config -c

- To edit Isconfig file:
    - litesoph config -e

5. Usage
    - To start gui application, use command
        - litesoph gui

6. To enable passwordless SSH

```
$ ls -al ~/.ssh/id_*.pub  #check existing key, if key exists goto step 2
$ ssh-keygen -t rsa      # Keep pressing enter
$ ssh-copy-id username@hostname -p xxxx   #Enter the password
```

Get the path of private key file

```
$ realpath ~/.ssh/id_rsa
```