Using ATSUP

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Notes by Jayson (May 31, 2022)

1 Installing Necessary Tools

There are a few tools and libraries that are necessary to run ATSUP. In order to install these, you must have access to a linux command line. Apple computers already have this in the Terminal application. To install it on a Windows computer, you must follow the instructions under "Installing the Linux Subsystem for Windows". The rest of the tutorial assumes that you have access to a Linux command line, and that you have ATSUP downloaded and unzipped.

1. Open the Linux terminal. On Apple this is just "Terminal", and on Windows this is "Windows Terminal", and you have to open an "Ubuntu" (or whatever version of Linux you installed) tab. Then navigate to wherever you unzipped "atsup-master".

2. To make sure Linux has the latest information about packages, type

```
sudo apt-get update
sudo apt-get upgrade
```

3. To install BLAS and LAPACK:

```
sudo apt-get install libblas-dev liblapack-dev
```

4. To install fftw3:

```
sudo apt-get install fftw3
```

5. To install sphinx:

```
sudo apt-get install python3-sphinx
```

6.1 Installing Cmake (according to the internet)

./bootstrap

make

make install

I remember to type something like: sudo apt-get install cmake ,but I don't know if that works;

6.2 For some reason when I tried to do cmake .. I was getting an error (CMAKE_CXX_COMPILER-NOTFOUND); I fixed using the following command:

sudo apt-get update && sudo apt-get install build-essential

6. To install gfortan and gcc (Fortran and C compilers)

```
sudo apt-get install gfortran
sudo apt-get install gcc
```

A good way to check if something is installed is to type

```
which [Library_name]
```

For example, if you want to find where cmake is installed, type

```
which cmake
```

2 Building the Documentation

The creators of ATSUP made documents that explain how ATSUP works, but to read them, you have to use sphinx to first build them.

```
cd /atsup-master/doc
make html
```

This builds several HTML documents in the /atsup-master/doc/build/html folder. The "tutorials.html" file contains directions on how to create the atsup_input and POSCAR files.

3 Running ATSUP

1. Navigate to the atsup-master directory
2. Type the following commands:

```
mkdir build
cd build
cmake ..
make
```

3. Create the input_atsup and POSCAR files, and place them in the atsup-master directory. **Do this after step 2.**
4. Now navigate to the atsup-master folder and type

```
python3 run_atsup.py
```

I had an error(NameError could not find input_atsup)

Solution: the input files should not have a txt extension

5. The results can be found in

```
/atsup-master/output
```

4 Installing the Linux Subsystem for Windows

1. Open **Control Panel**
2. Navigate to **Programs**
3. Click on **Turn Windows features on or off**
4. Check **Windows Subsystem for Linux**
5. Click **OK** and then **Restart Now**

I had to install ubuntu from the Microsoft store , and it seems like with that is no necessary to do 4.1.
I remember to type bash in a windows terminal to access to the ubuntu terminal

4.1 Starting a Linux Session

1. Open **Windows Terminal**
2. Click on the down arrow at the top and click **Ubuntu**
3. To navigate to your Desktop, type the command:

```
cd /mnt/c/Users/|Your_Username|/Desktop
```

If you don't know how to navigate using a terminal:
cd < new directory> : changes the directory to < new directory>
mkdir <name>: creates a new directory with the name <name>
cd .. : goes to a previous directory or one level up
These are the ones that you should know and use the most, but there are more. For more information look for linux commands on the internet.

If you have questions, you can contact me: jayson.has@gmail.com