#### Installation of visualization tools in Ubuntu-20.04

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If you have recently installed Ubunutu20.04 and you want to install various visualization tools. Follow the procedure mentioned below.

- # Update your Ubuntu-20.04 operating system
- \$ sudo apt-get update
- # Install some more required pakages before installing DFT visualization tools.
- \$ sudo apt-get install make
- \$ sudo apt-get install cmake
- \$ sudo apt-get install m4
- \$ sudo apt-get install gcc
- \$ sudo apt-get install g++
- \$ sudo apt-get install gfortran

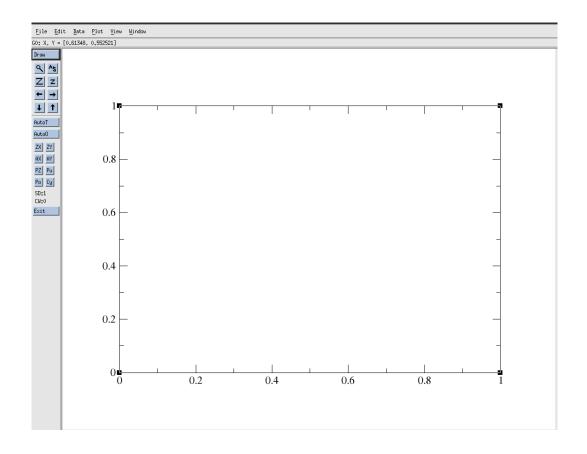
Now you can install required visualization tools using single command.

# (1) Install Xmgrace (<a href="https://plasma-gate.weizmann.ac.il/Grace/">https://plasma-gate.weizmann.ac.il/Grace/</a> ): a plotting tool \$ sudo apt-get install grace

Check whether xmgrace is installed or not using command:

\$ xmgrace

You will get:



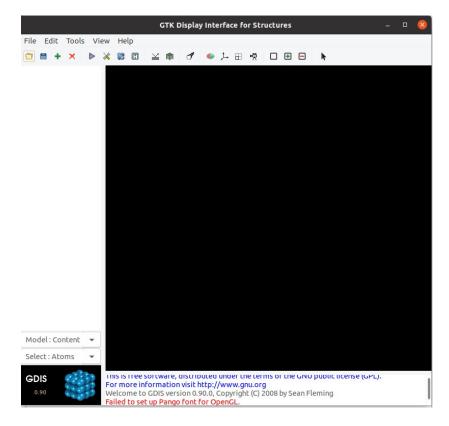
## (2) Install gdis (<a href="http://gdis.seul.org/">http://gdis.seul.org/</a>)

\$ sudo apt-get install gdis

Check whether gdis is installed or not using command:

\$ gdis

You will get:



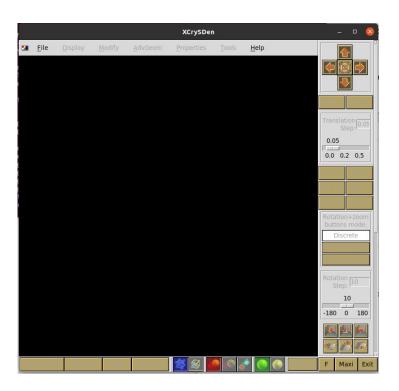
## (3) Install Xcrysden (<a href="http://www.xcrysden.org/">http://www.xcrysden.org/</a>)

\$ sudo apt-get install xcrysden

Check whether xcrysden is installed or not using command:

\$ xcrysden

You will get:



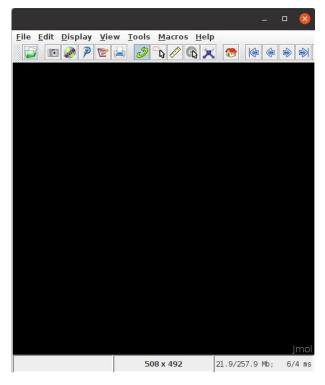
### (4) Install Jmol (<a href="https://jmol.sourceforge.net/">https://jmol.sourceforge.net/</a>)

\$ sudo apt-get install jmol

Check whether jmol is installed or not using command:

\$ jmol

You will get:



## (5) Install Molden (<a href="https://www.theochem.ru.nl/molden/">https://www.theochem.ru.nl/molden/</a>)

\$ sudo apt install snapd

\$ sudo snap install molden

Check whether Molden is installed or not using command:

\$ molden

You will get:



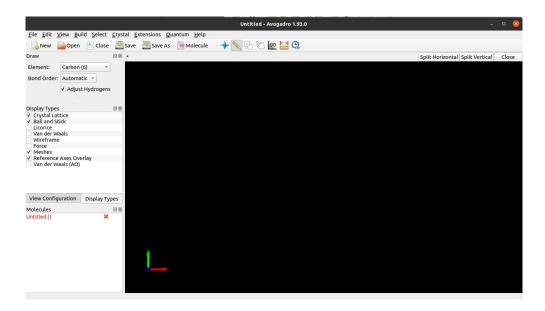
#### (6) Install Avogadro2 (<a href="https://avogadro.cc/">https://avogadro.cc/</a>)

\$ sudo apt-install avogadro2

Check whether avogadro2 is installed or not using command:

\$ avogadro2

You will get:



#### (6) Install VESTA (<a href="https://jp-minerals.org/vesta/en/">https://jp-minerals.org/vesta/en/</a>)

In order to install VESTA in ubuntu20.04 please follow the given commands in sequence.

Open the VESTA software link <a href="https://jp-minerals.org/vesta/en/download.html">https://jp-minerals.org/vesta/en/download.html</a> and download \*.rpm file for linux. The latest version is vesta-3.5.8-1.x86\_64.rpm Now install this vesta-3.5.8-1.x86 64.rpm file using following commands:

- # Add the Universe Repository
- \$ sudo add-apt-repository universe
- # Update apt-get
- \$ sudo apt-get update

Install Alien package

\$ sudo apt-get install alien

Convert .rpm package to .deb

\$ sudo alien vesta-3.5.8-1.x86 64.rpm

This command will give a vesta\_3.5.8-2\_amd64.deb file. Install this Converted Package

\$ sudo dpkg -i vesta\_3.5.8-2\_amd64.deb

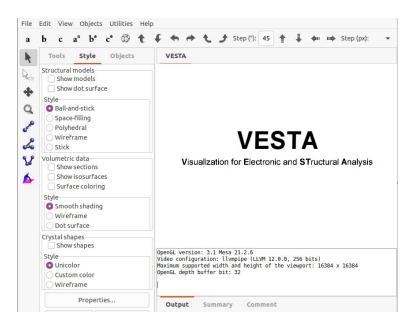
One can also use rpm file directly to install in ubuntu using the command

\$ sudo alien -i vesta-3.5.8-1.x86 64.rpm

Now VESTA is ready to use VESTA. Now open the VESTA using the command

#### **\$ VESTA**

you will get:



(7) Install wine (<a href="https://utho.com/docs/tutorial/how-to-install-wine-on-ubuntu-20-04/">https://utho.com/docs/tutorial/how-to-install-wine-on-ubuntu-20-04/</a>)

If you want to use some window based software in your linux operating system you should have wine software in your ubunutu20.04. Which can be easilty installed using command

\$ sudo apt install wine64

Now you can enjoy learning visualization tools to get your DFT based results.

Thanking You.

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