# Computational chemistry job automation workshop

## Requirements:

1. **A machine running Ubuntu (20.04 LTS preferred):**
   If you do not have Ubuntu machine, try installing one on Virtual box. To install Ubuntu on Virtual Box, the following resources are useful –
   - https://www.youtube.com/watch?v=x5MhydijWmc
   - https://www.wikihow.com/Install-Ubuntu-on-VirtualBox
   - https://itsfoss.com/install-linux-in-virtualbox/

   Try to get Ubuntu 20.04 LTS version while installing. The resources may use some other versions.

2. **MongoDB:**
   MongoDB community edition will be used to store data to run the computation jobs as well as the processed data. Follow the instructions on the MongoDB website to install - https://docs.mongodb.com/v4.4/tutorial/install-mongodb-on-ubuntu/. You will only need steps 1-4 under "Installing MongoDB Community Edition" and steps 1-2 for "Run MongoDB Community Edition"

3. **Miniconda:**
   We will use the conda package manager in this workshop. You can download the Linux installer from the link below –
   https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh

   To install first change the permission to make it executable then run the bash script in the terminal

   ```
   chmod +x Miniconda3-latest-Linux-x86_64.sh
   bash Miniconda3-latest-Linux-x86_64.sh
   ```

4. **(Optional) PyCharm:**
   You can install PyCharm IDE professional edition if you in academia. In that case you can need to register with your institution email and download the professional edition. Else, you can download the community edition for Linux from here
   https://www.jetbrains.com/pycharm/download/other.html

If you have a macOS, you do not need to install virtual box. However, you would still need MongoDB and Miniconda which can be downloaded from the following links and follow the instructions.

MongoDB- https://docs.mongodb.com/manual/tutorial/install-mongodb-on-os-x/

Miniconda - https://repo.anaconda.com/miniconda/Miniconda3-latest-MacOSX-x86_64.sh