# Installation and Configuration of LAMMPS Using CMake

## 1. Prerequisites

Dear students, before starting the installation process, ensure the following packages are installed on your system. Use the following command to install them:

```
sudo apt update
sudo apt install -y build-essential cmake g++ gfortran git \
  libfftw3-dev libjpeg-dev libpng-dev libhdf5-dev libopenmpi-dev \
  liblapack-dev libblas-dev libpython3-dev libcurl4-openssl-dev \
  libzstd-dev gedit
```

### Common Issues During Configuration

- Missing libraries such as `libkim-api.so` or `libhdf5`. Make sure these libraries are also installed. - Conflicts with Conda libraries. Use a non-Conda shell during configuration if needed.

**Note:** This list covers common dependencies needed for LAMMPS. If you enable additional packages (e.g., KIM or Voronoi), ensure their dependencies are installed. You can install these easily by using `sudo apt install package_name` command.

## 2. Download and Setup LAMMPS

Clone the LAMMPS repository and prepare the build directory:

```
# Clone the LAMMPS repository
git clone https://github.com/lammps/lammps.git
cd lammps

# Create a build directory
mkdir build
cd build
```

## 3. Configure LAMMPS with CMake

While being within the build directory you would need to use cmake

```
ccmake ../cmake
```

this command will lead to run cmake while copying the cmake.txt file from the cmake (".. cmake" part of the last command) directory already available in the downloaded lammps folder.

Now please press the **"c"** button it will configure and then press **"e"** button to remake the configuration and click enter on the packages which you want to install and again press **"c"** to configure once all the necessary packages listed below are made **"on"**.

Note: Please avoid every module package enabling for the installation. You would just need to make these packages "on" by clicking the enter button, where the list is given below...

### Required LAMMPS Packages

ASPHERE ATC AWPMD BOCS BODY CG-DNA CG-SPICA CLASS2 COLLOID COMPRESS CORESHELL DI-ELECTRIC DIFFRACTION DIPOLE DPD-BASIC DPD-MESO DPD-REACT DPD-SMOOTH DRUDE EFF ELECTRODE EXTRA-PAIR FEP GRANULAR H5MD KIM KSPACE LAT-BOLTZ MANIFOLD MANYBODY MC MEAM MGPT MISC MOFFF MOLECULE MOLFILE NETCDF OPENMP OPT ORIENT PERI PHONON POEMS PYTHON QEQ QTB REPLICA RIGID SHOCK SMTBQ SPH SRD TALLY UEF VORONOI

The 'CMAKE_INSTALL_PREFIX' specifies where LAMMPS will be installed. If the configuration fails, ensure that all required dependencies (see Section 1) are installed.

## 4. Build and Install LAMMPS

Compile and install LAMMPS:

```
make -j$(nproc)     # Compile using all available cores
make install        # Install to the specified directory
```

## 5. Make LAMMPS Executable Globally Available

To make the LAMMPS executable accessible from any directory:

1. Add the installation directory to your `PATH` variable. Edit your `~/.bashrc` file:

   ```
   nano ~/.bashrc
   ```

   You can also use **gedit** command to open which would be easier to edit and save due to the user interface.

   ```
   gedit ~/.bashrc
   ```

2. Add the following line at the end of the file:

   ```
   export PATH=$PATH:/home/yourcomputername/user/local/bin
   export PATH=$PATH:~/user/local/bin
   export LD_LIBRARY_PATH=$LD_LIBRARY_PATH:/home/yourcomputername/
      lammps/build/kim_build-prefix/lib
   ```

   **Caution:** Please replace "yourcomputername" with your own computer name.

3. Save and exit the editor. Then reload the `.bashrc` file:

   ```
   source ~/.bashrc
   ```

**Test the Setup:** Run the following command to verify:

```
lmp -h
```

This should display the help information for the LAMMPS executable.

## 6. Notes on Using LAMMPS with Conda

If you are using Conda, you may encounter library conflicts. To avoid this:

1. Either deactivate Conda before running LAMMPS:

```
conda deactivate
```

2. Or ensure that the correct library paths are loaded by setting:

```
export LD_LIBRARY_PATH=/home/yourcomputername/user/local/lib:
   $LD_LIBRARY_PATH
```

## 7. Summary

This guide provides a step-by-step process to install LAMMPS using CMake, resolve common issues, and configure the environment for ease of use. If you encounter additional issues, refer to the LAMMPS documentation or community forums for support.

## 8. In case of failure

Take help from the **C H A T G P T** (free version can make it through). Follow step by step and carefully read the error message. Do not give up until installed and executable globally (from any directory) within the home environment.