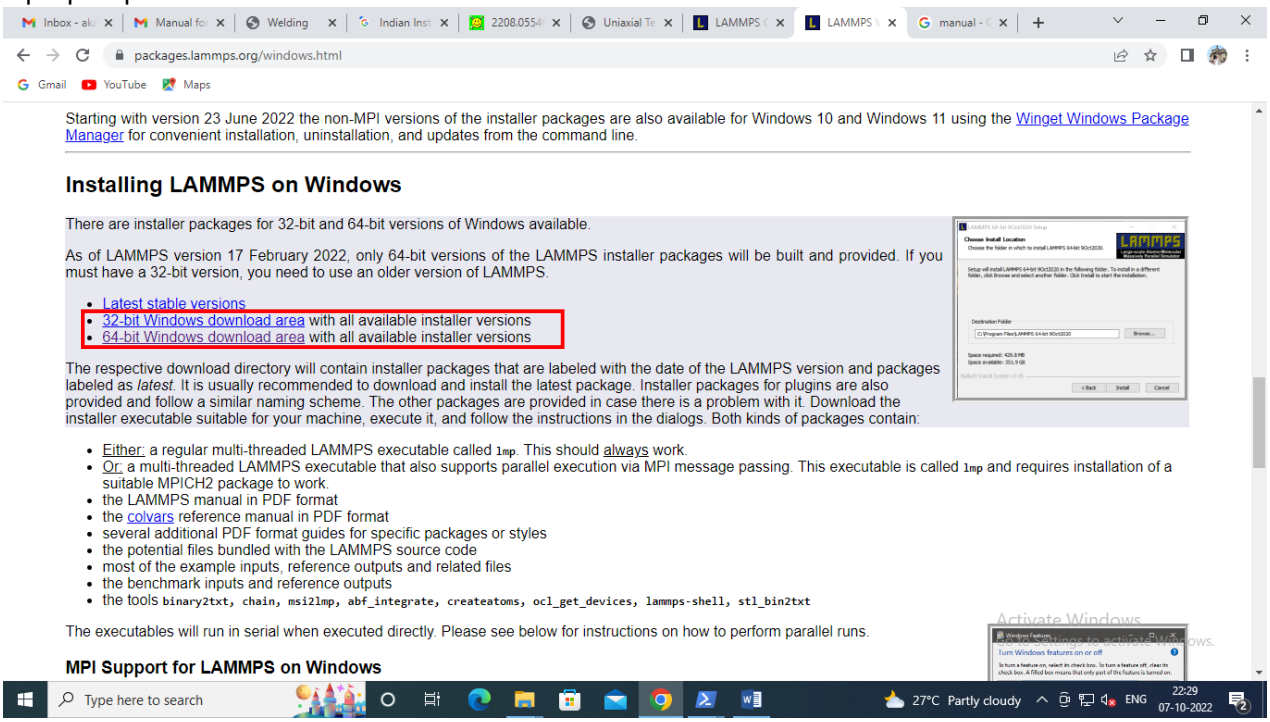
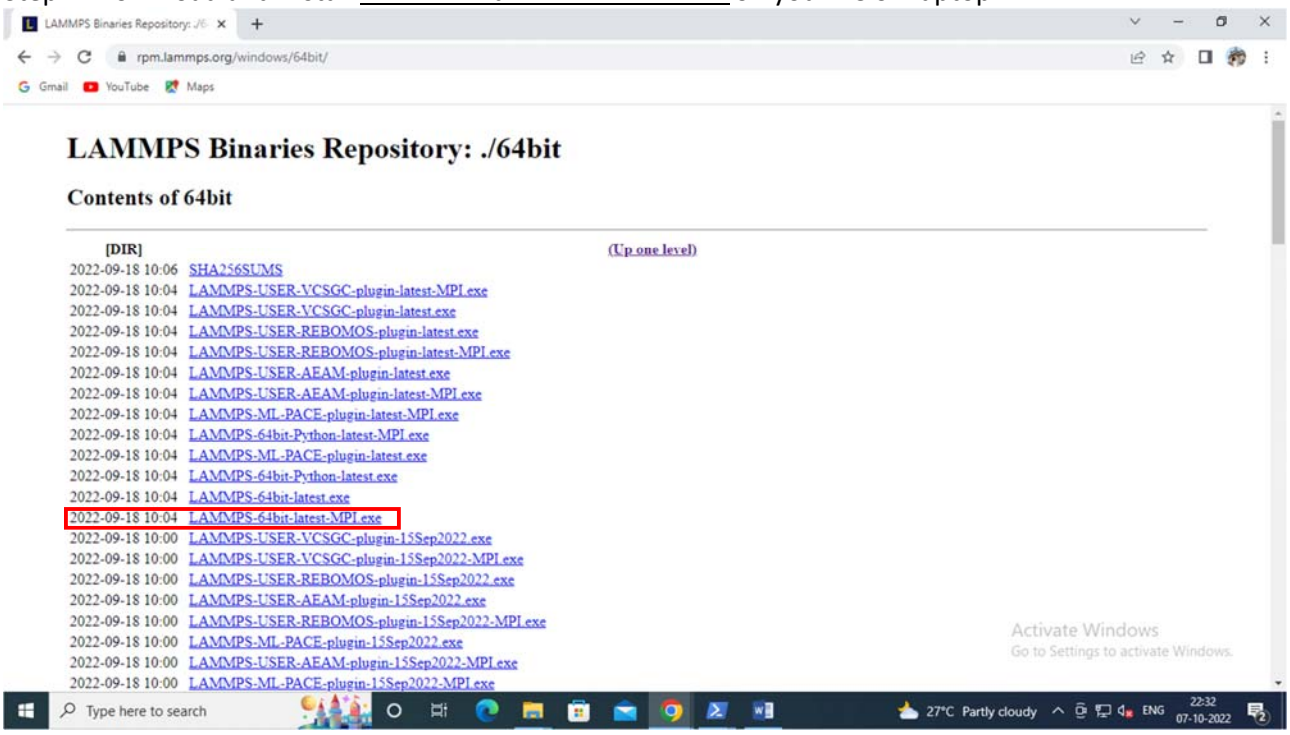
LAMMPS-MPI Installation Manual

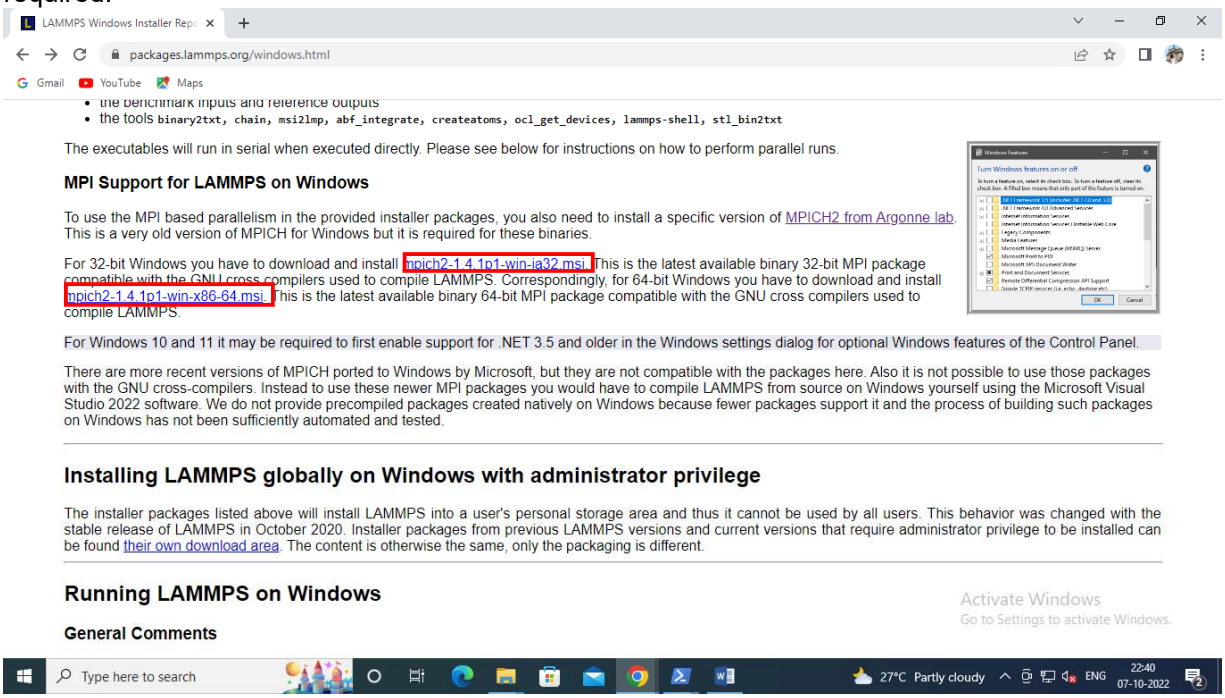
Step 1: Open the link https://packages.lammps.org/windows.html and go to Installing LAMMPS on Windows then click on 64-bit Windows download area or 32-bit Windows download area as the PC or laptop required.



Step 2: Download and Install LAMMPS-64bit-latest-MPI.exe on your PC or Laptop.

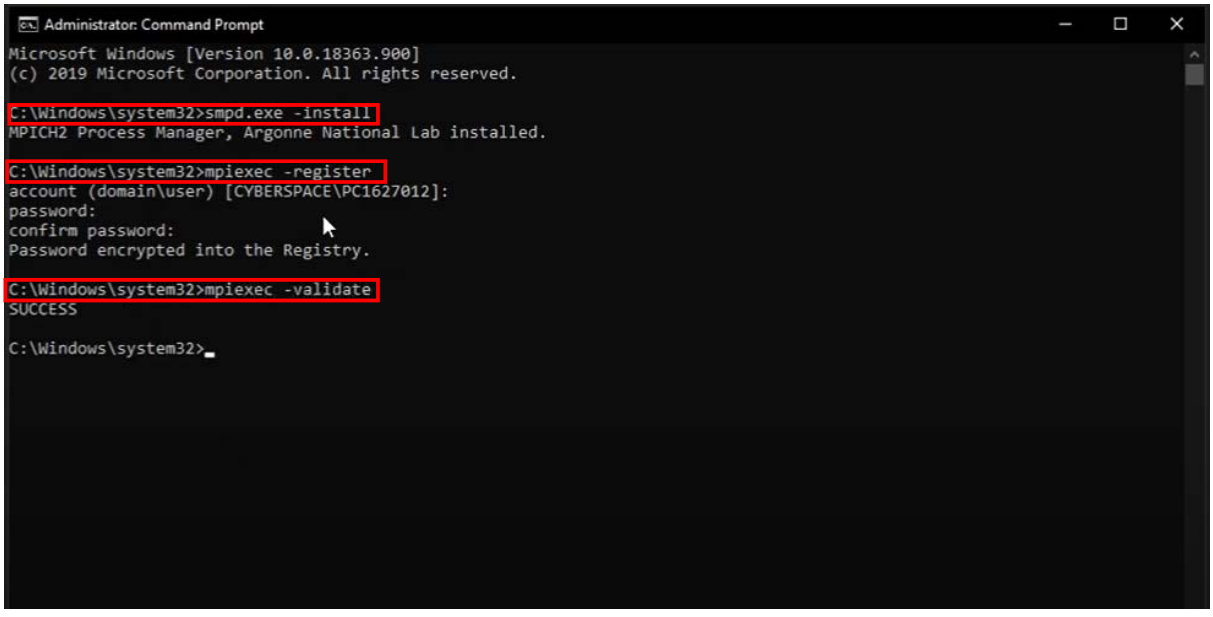


Step 3: After successfully installing the LAMMPS-64bit-latest-MPI.exe again open the link https://packages.lammps.org/windows.html and go to MPI Support for LAMMPS on Windows then download and install mpich2-1.4.1p1-win-x86-64.msi or mpich2-1.4.1p1-win-ia32.msi as your laptop or PC required.



Step 4: After installing mpich2-1.4.1p1-win-x86-64.msi run command prompt as administrator and follow the steps for cmd.

- Run smpd.exe -install
- Run mpiexec -register
  - In the "account:" just press enter
  - In the "password:" write the password of your pc (not pin)
  - write the password again
- Run mpiexec –validate



NOTE: For running LAMMPS-MPI on your system open the folder in which your input and potential files are there then open powershell or teminal and type ***mpiexec -np 4 lmp -in <inputfile>,*** Here, -np 4 is the number of processor which are going to be used for the simulation.