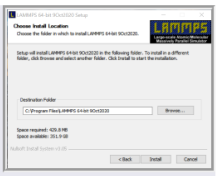
LAMMPS Installation Instructions

Step 1: Download the lammps installer from website.

https://packages.lammps.org/windows.html

Installing LAMMPS on Windows

There are installer packages for 32-bit and 64-bit versions of Windows available.



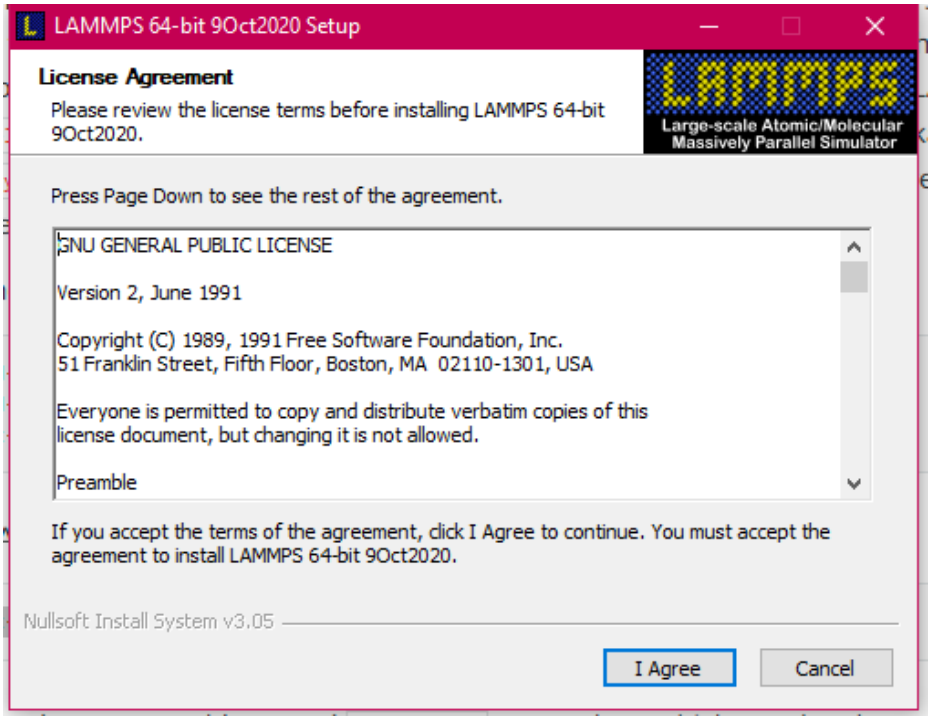
As of LAMMPS version 17 February 2022, only 64-bit versions of the LAMMPS installer packages will be built and provided. If you must have a 32-bit version, you need to use an older version of LAMMPS.

- Latest stable versions
- 32-bit Windows download area with all available installer versions
- 64-bit Windows download area with all available installer versions

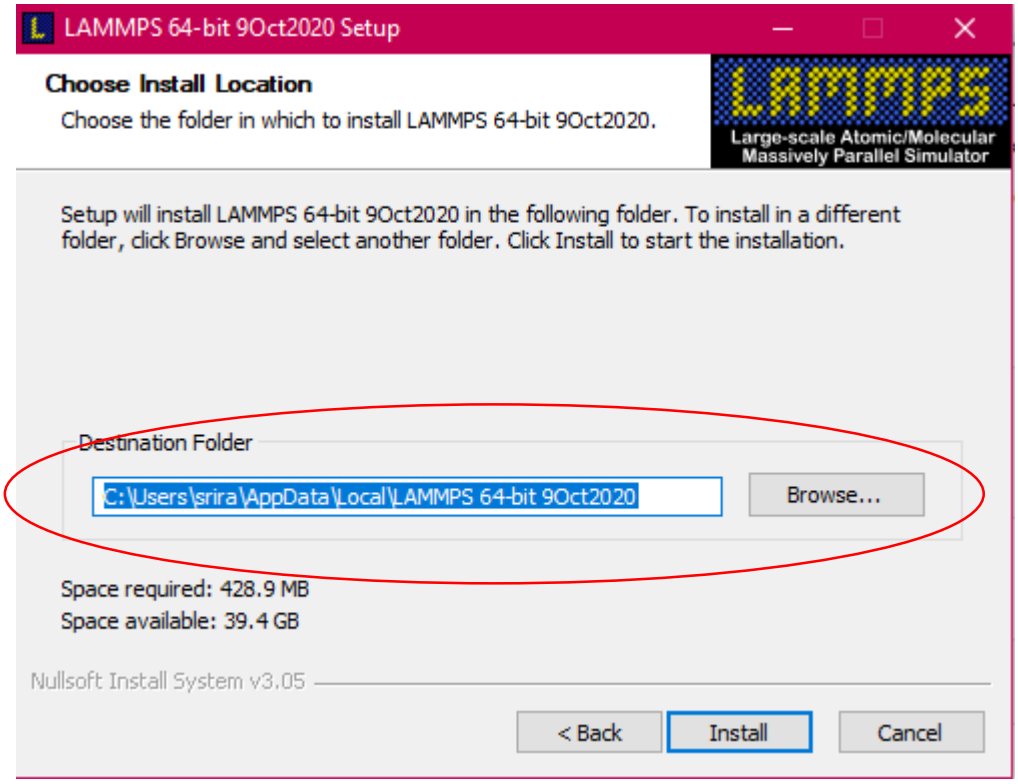
The respective download directory will contain installer packages that are labeled with the date of the LAMMPS version and packages labeled as *latest*. It is usually recommended to download and install the latest package. The other packages are provided in case there is a problem with it. Download the installer executable suitable for your machine, execute it, and follow the instructions in the dialogs. Each version will install into a different directory, so it is possible to have multiple versions installed at the same time (however it is not recommended). Both kinds of packages contain:

- Either: a regular multi-threaded LAMMPS executable called `lmp`. This should always work.
- Or: a multi-threaded LAMMPS executable that also supports parallel execution via MPI message passing. This executable is called `lmp` and requires installation of a suitable MPICH2 package to work.
- the LAMMPS manual in PDF format
- the colvars reference manual in PDF format
- several additional PDF format guides for specific packages or styles
- the potential files bundled with the LAMMPS source code
- most of the example inputs, reference outputs and related files
- the benchmark inputs and reference outputs
- the tools `binary2txt, chain, msi2lmp, abf_integrate, createatoms, ocl_get_devices, lammps-shell`

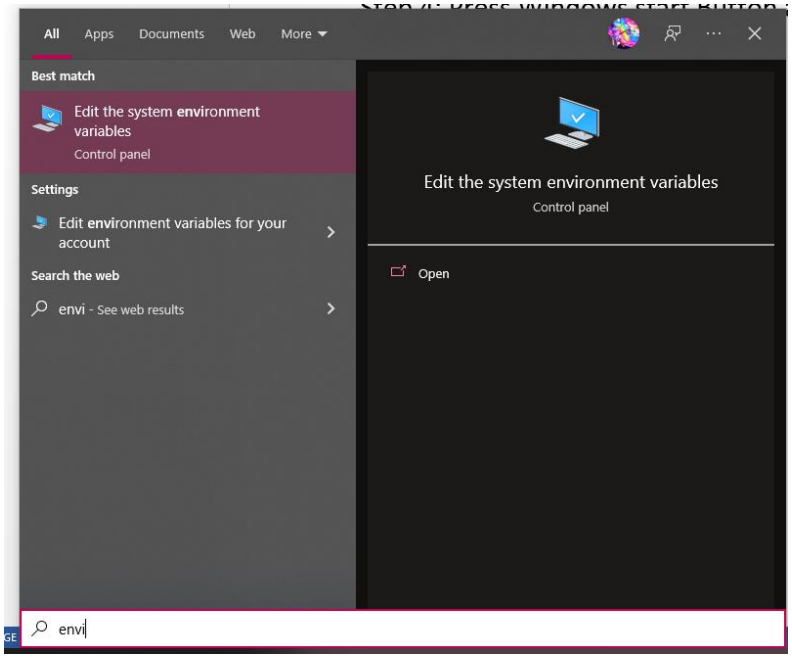
Step 2: Run the installer



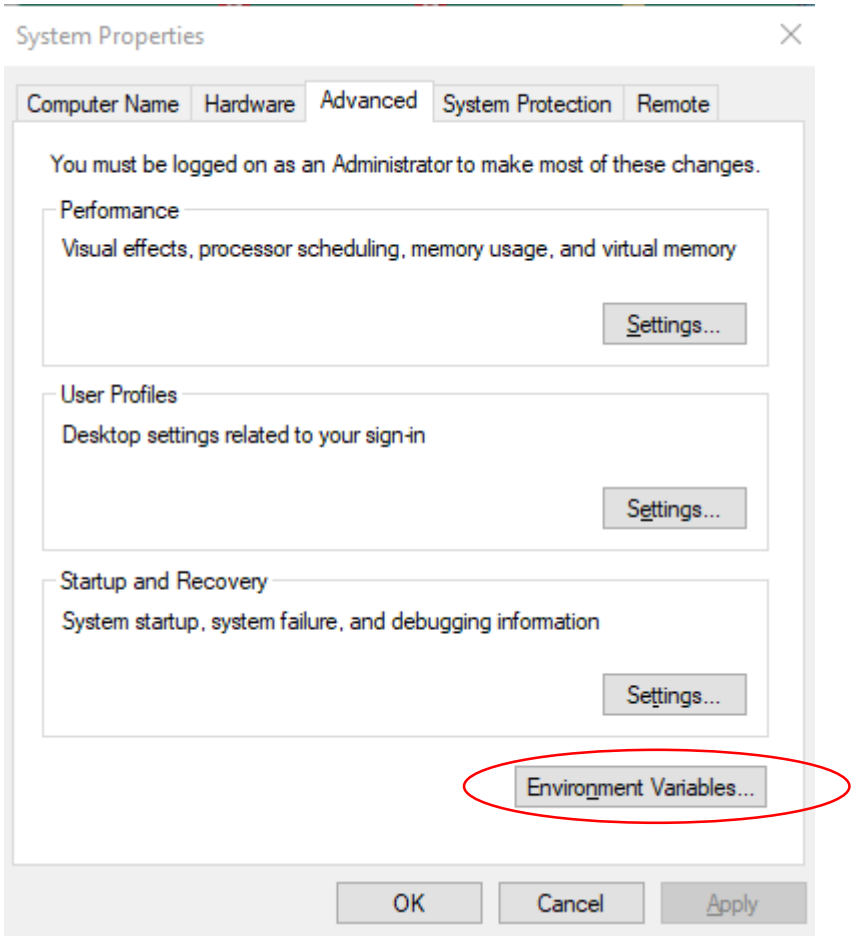
Step 3 : Copy or remember the path where LAMMPS will be installed



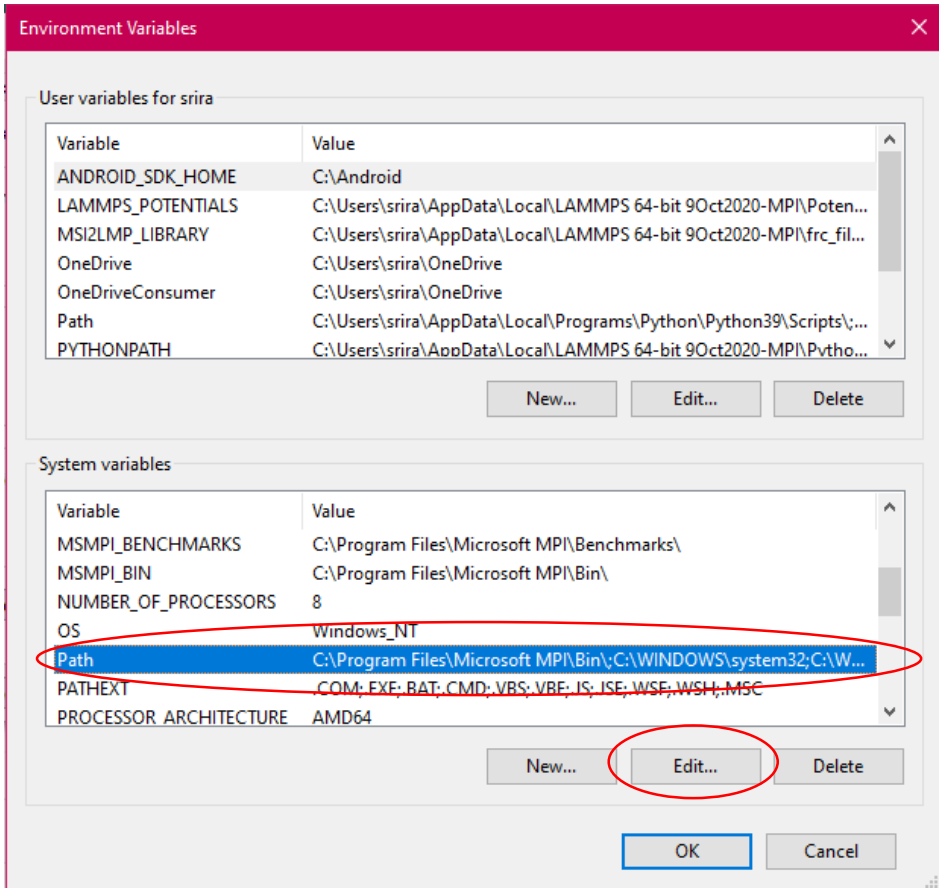
Step 4: Press Windows start Button and type environment



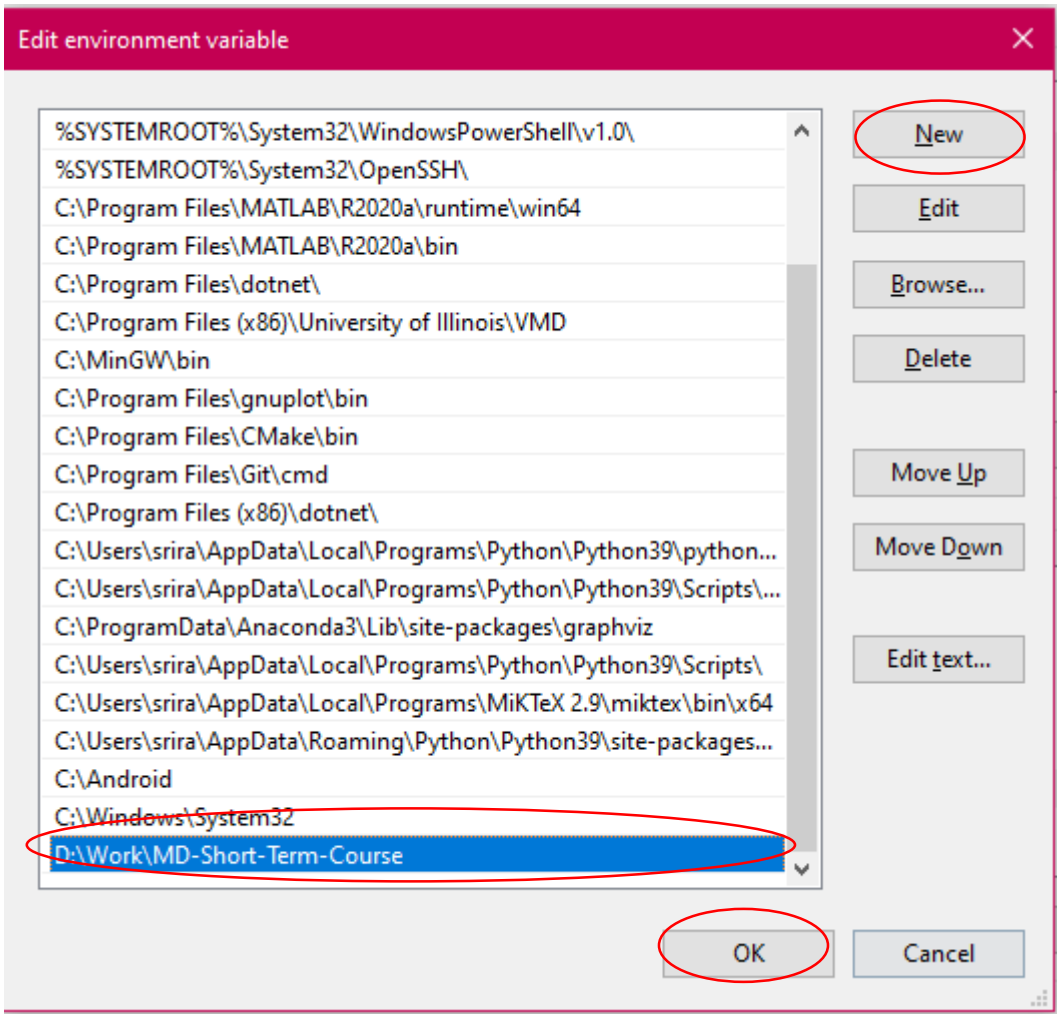
Step 5 : Open the Edit the System Environment Variables tab and click on Environment Variables



Step 6: Find the path variable in System Variables and click edit



Step 7 Click on New and Copy the path there and click Ok



Step 8: Go to desktop, Press shift and right-click and open a Powershell Terminal. Type lmp_serial.exe –help

If the installation was correct, you should see something like this: