

LAMMPS Installation Instructions

Step 1: Download the lammmps installer from website.

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

Installing LAMMPS on Windows

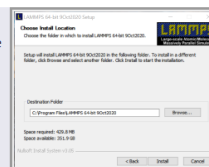
There are installer packages for 32-bit and 64-bit versions of Windows available.

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.

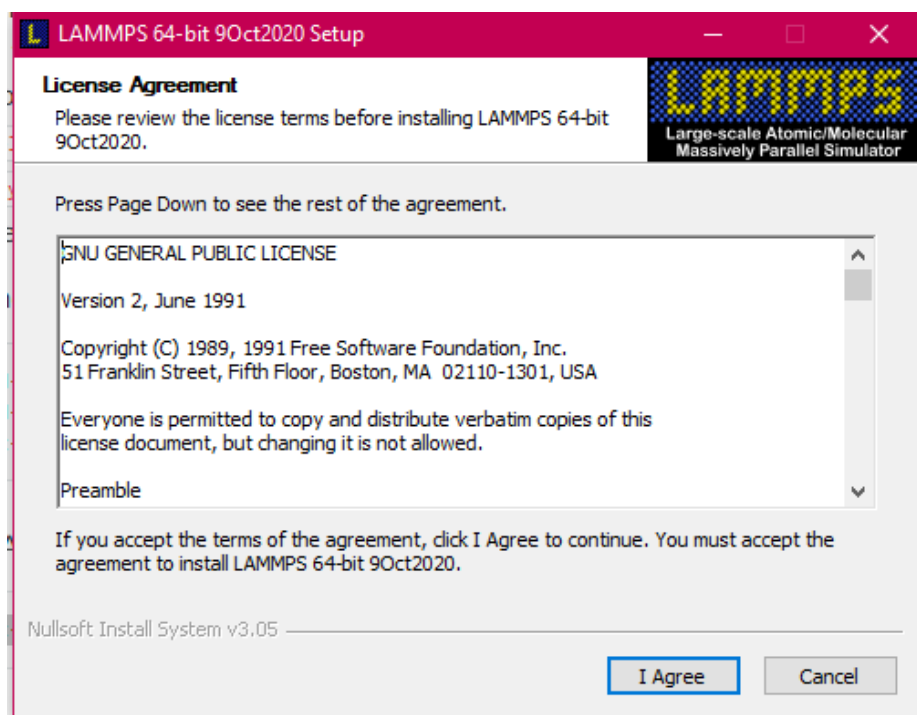
- [Latest stable versions](#)
- [32-bit Windows download area](#) with all available installer versions
- [64-bit Windows download area](#) with all available installer versions

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:

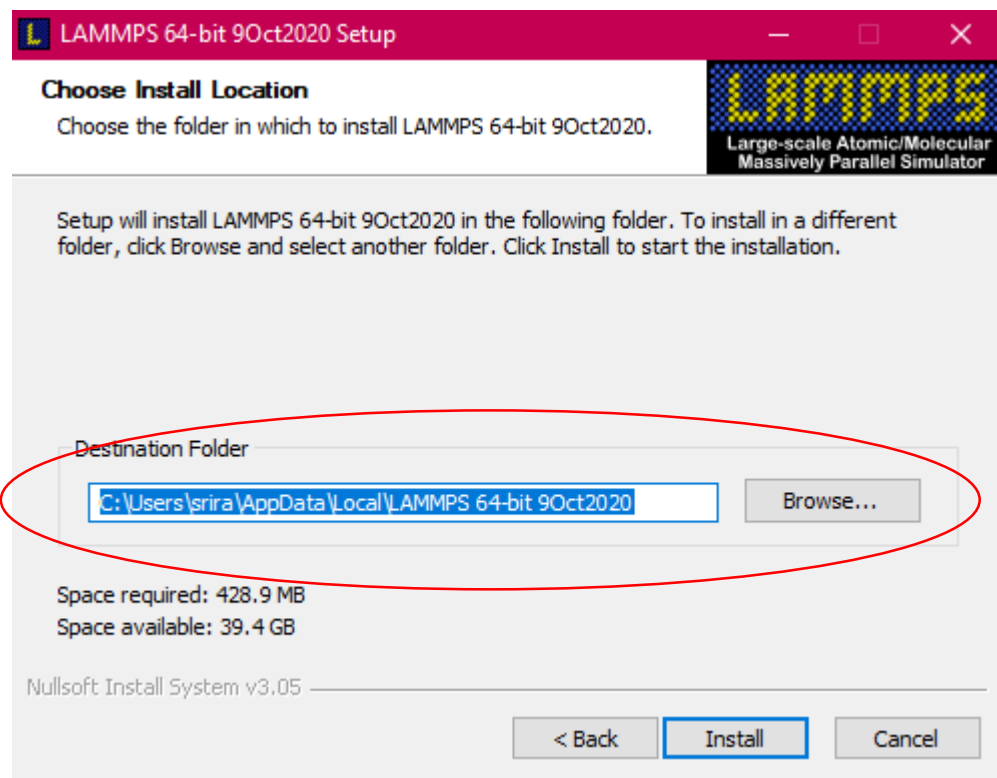
- Either: a regular multi-threaded LAMMPS executable called `lmp`. This should always work.
- Or: a multi-threaded LAMMPS executable that also supports parallel execution via MPI message passing. This executable is called `lmp` and requires installation of a suitable MPICH2 package to work.
- the LAMMPS 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`



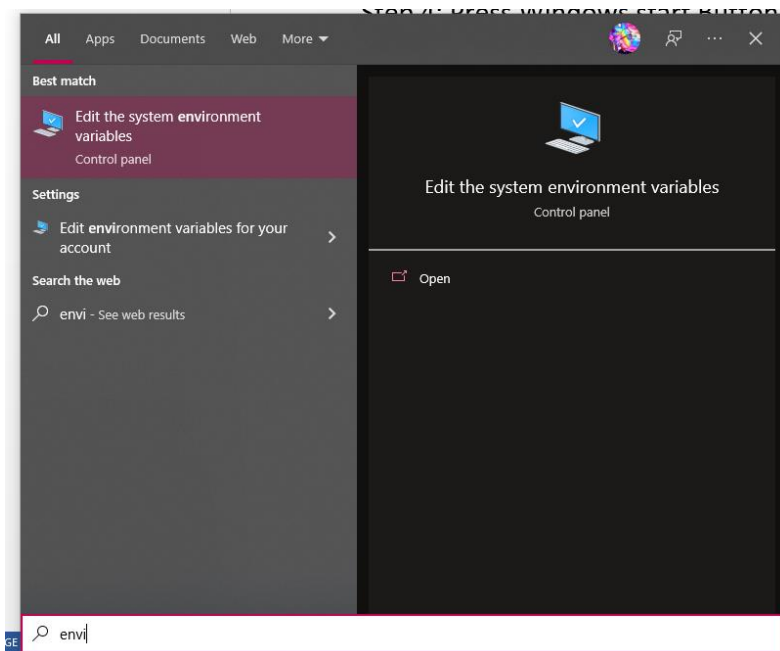
Step 2: Run the installer



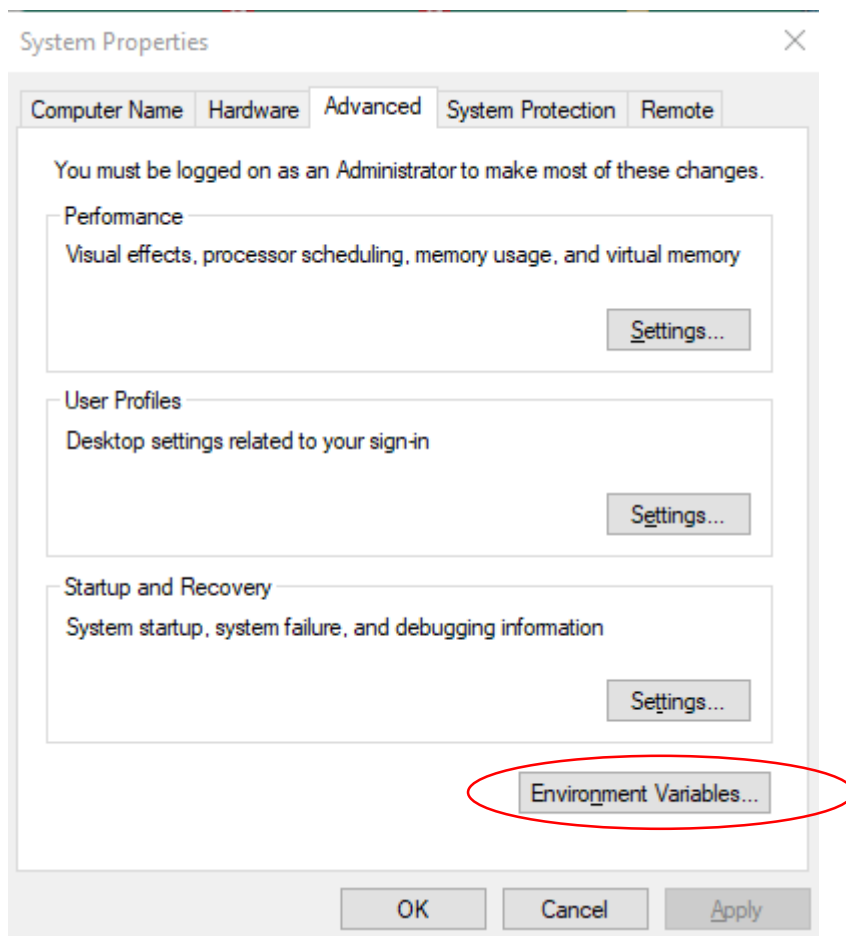
Step 3 : Copy or remember the path where LAMMPS will be installed



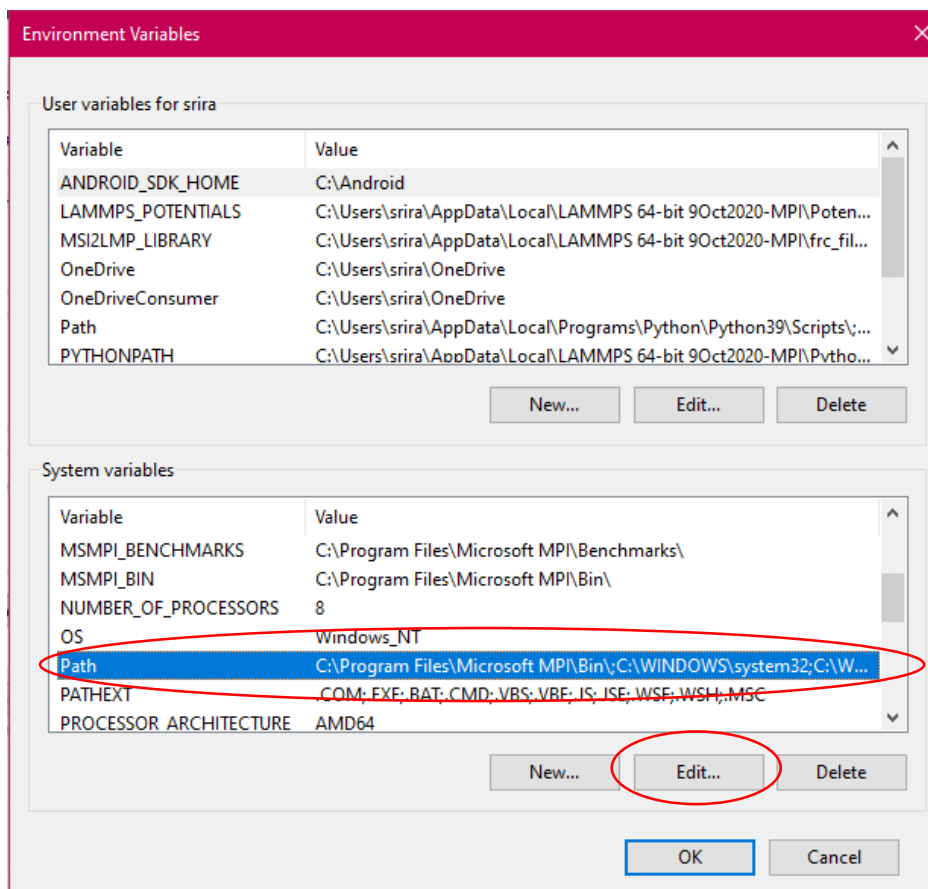
Step 4: Press Windows start Button and type environment



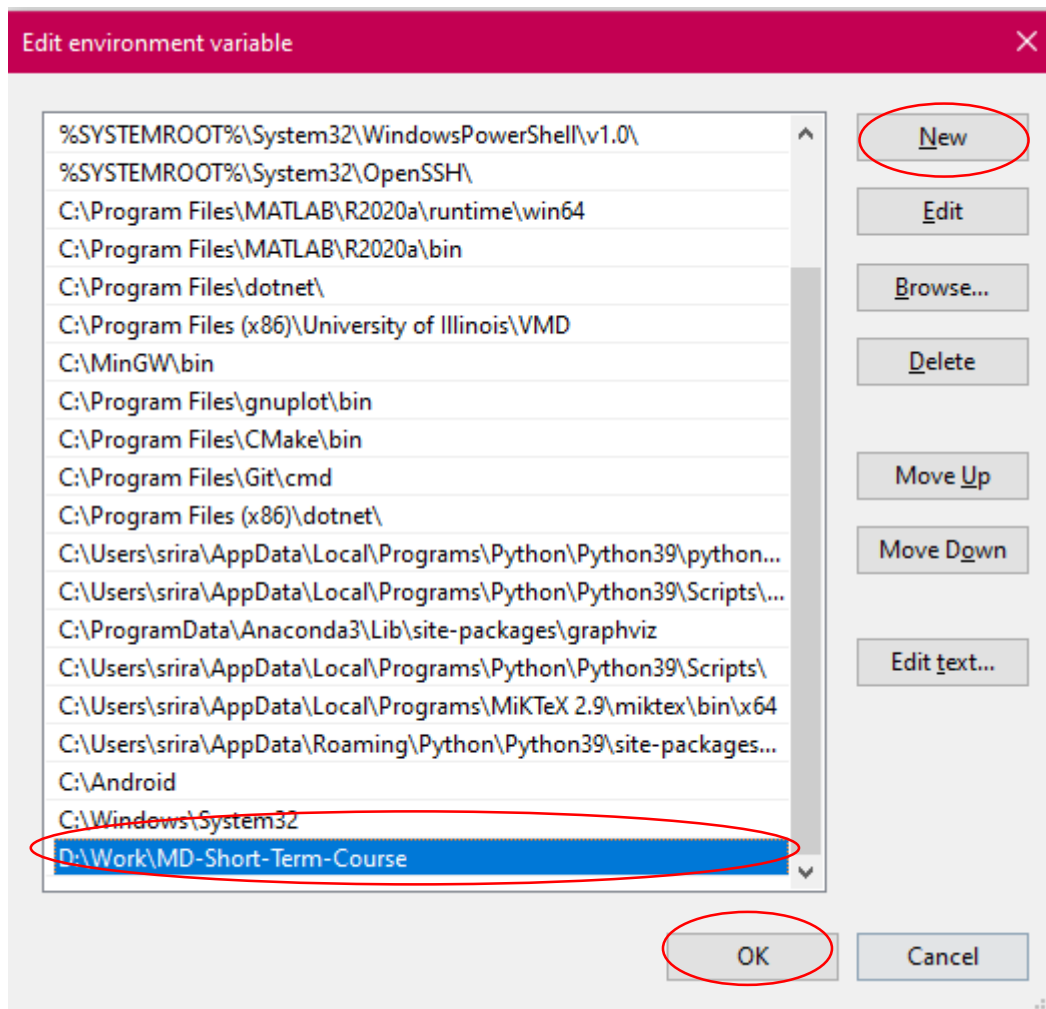
Step 5 : Open the Edit the System Environment Variables tab and click on Environment Variables



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

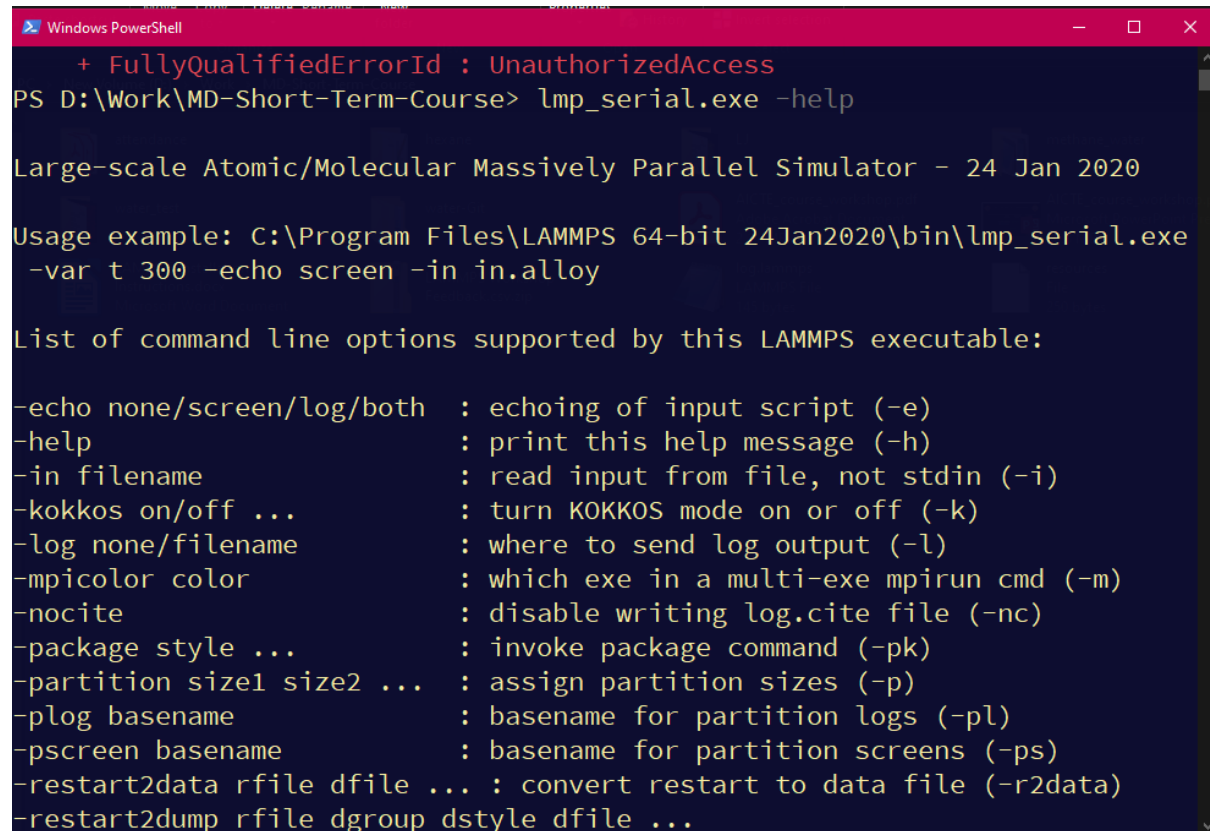


Step 7 Click on New and Copy the path there and click Ok



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:



```
Windows PowerShell
+ FullyQualifiedErrorId : UnauthorizedAccess
PS D:\Work\MD-Short-Term-Course> lmp_serial.exe -help

Large-scale Atomic/Molecular Massively Parallel Simulator - 24 Jan 2020

Usage example: C:\Program Files\LAMMPS 64-bit 24Jan2020\bin\lmp_serial.exe
-var t 300 -echo screen -in in.alloy

List of command line options supported by this LAMMPS executable:

-echo none/screen/log/both : echoing of input script (-e)
-help                      : print this help message (-h)
-in filename               : read input from file, not stdin (-i)
-kokkos on/off ...        : turn KOKKOS mode on or off (-k)
-log none/filename        : where to send log output (-l)
-mpicolor color           : which exe in a multi-exe mpirun cmd (-m)
-nocite                   : disable writing log.cite file (-nc)
-package style ...        : invoke package command (-pk)
-partition size1 size2 ... : assign partition sizes (-p)
-plog basename            : basename for partition logs (-pl)
-pscreen basename         : basename for partition screens (-ps)
-restart2data rfile dfile ... : convert restart to data file (-r2data)
-restart2dump rfile dgroup dstyle dfile ...
```