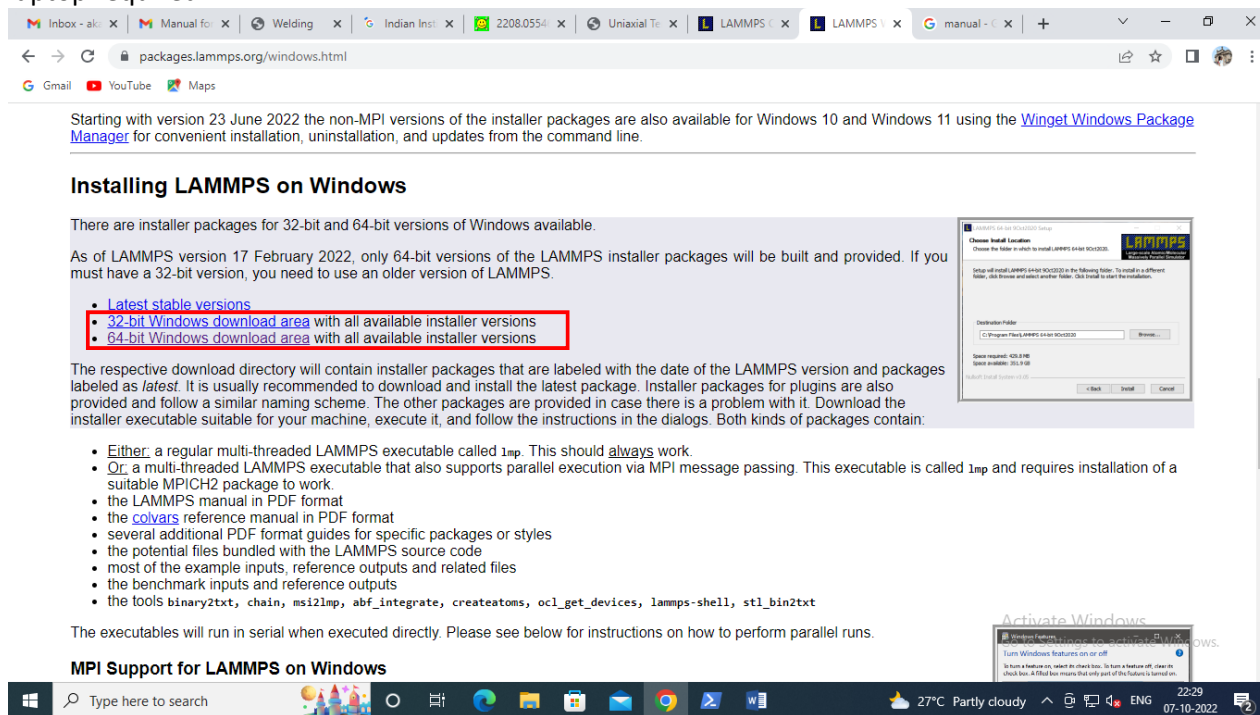


LAMMPS-MPI Installation Manual

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.



Starting with version 23 June 2022 the non-MPI versions of the installer packages are also available for Windows 10 and Windows 11 using the [Winget Windows Package Manager](#) for convenient installation, uninstallation, and updates from the command line.

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

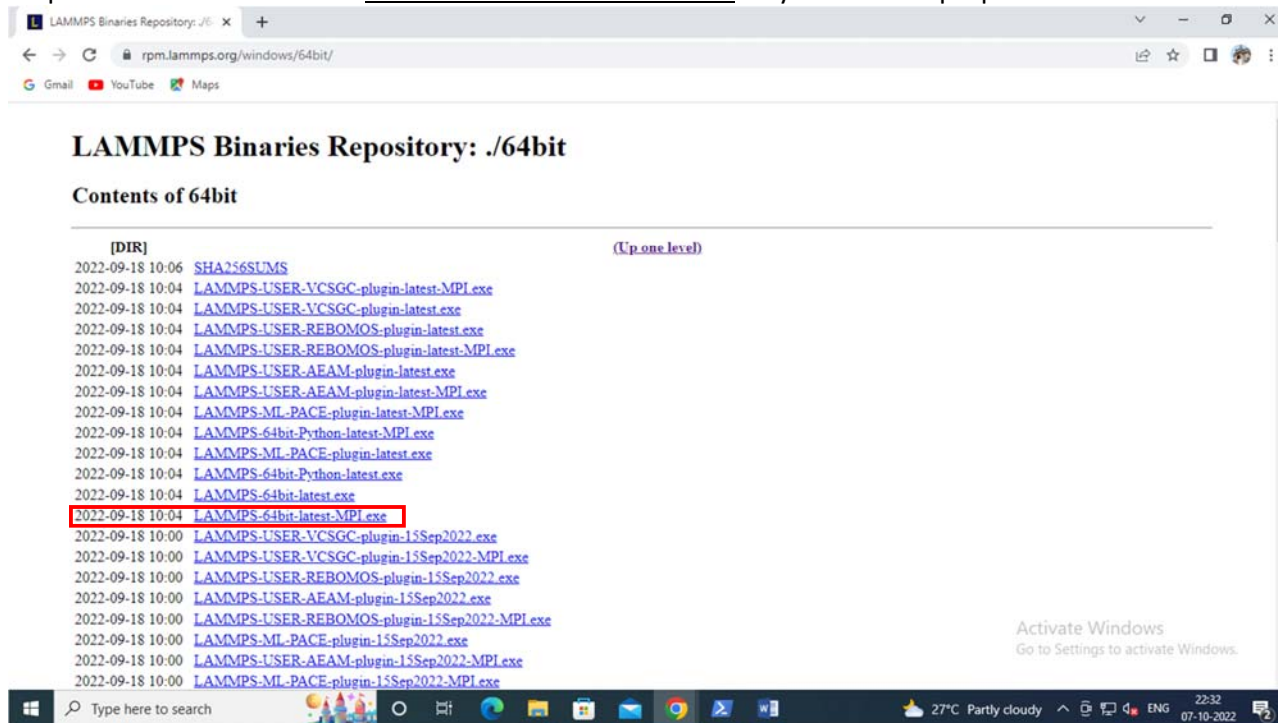
The respective download directory will contain installer packages that are labeled with the date of the LAMMPS version and packages labeled as *latest*. It is usually recommended to download and install the latest package. Installer packages for plugins are also provided and follow a similar naming scheme. 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. 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`, `createtoms`, `ocl_get_devices`, `lammps-shell`, `stl_bin2txt`

The executables will run in serial when executed directly. Please see below for instructions on how to perform parallel runs.

MPI Support for LAMMPS on Windows

Step 2: Download and Install [LAMMPS-64bit-latest-MPI.exe](#) on your PC or Laptop.



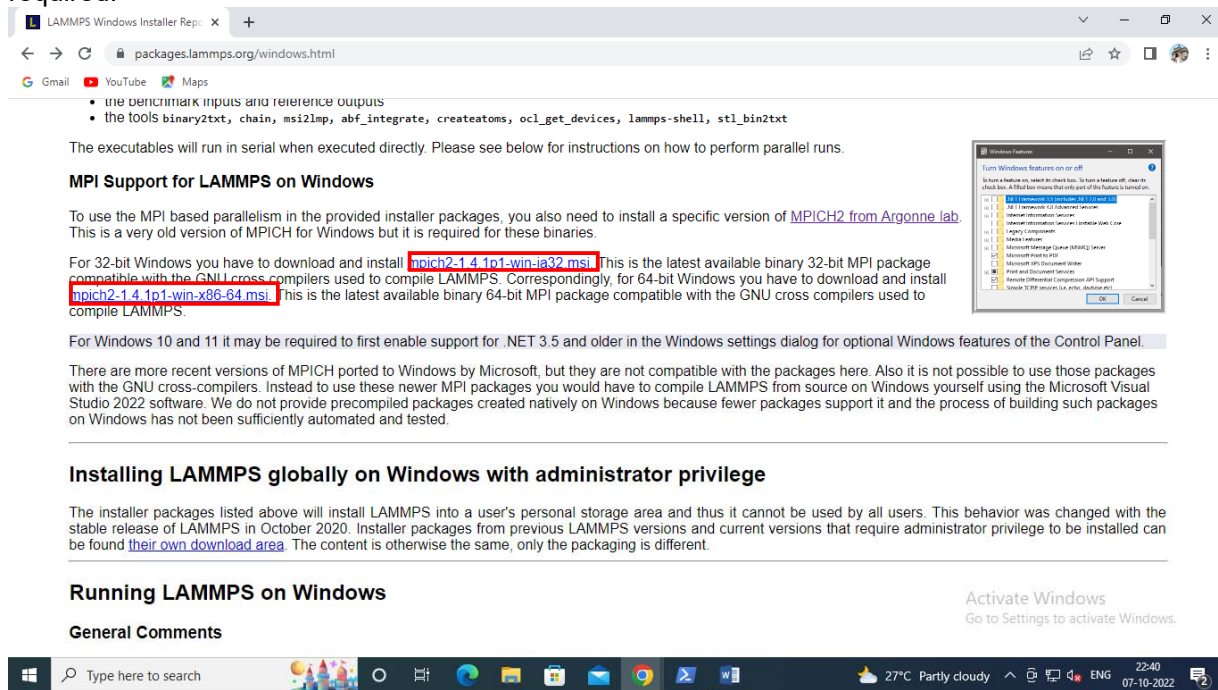
LAMMPS Binaries Repository: ./64bit

Contents of 64bit

[\(Up one level\)](#)

Timestamp	SHA256 Hash	File Name
2022-09-18 10:06	SHA256SUMS	
2022-09-18 10:04		LAMMPS-USER-VCSGC-plugin-latest-MPI.exe
2022-09-18 10:04		LAMMPS-USER-VCSGC-plugin-latest.exe
2022-09-18 10:04		LAMMPS-USER-REBOMOS-plugin-latest.exe
2022-09-18 10:04		LAMMPS-USER-REBOMOS-plugin-latest-MPI.exe
2022-09-18 10:04		LAMMPS-USER-AEAM-plugin-latest.exe
2022-09-18 10:04		LAMMPS-USER-AEAM-plugin-latest-MPI.exe
2022-09-18 10:04		LAMMPS-ML-PACE-plugin-latest-MPI.exe
2022-09-18 10:04		LAMMPS-64bit-Python-latest-MPI.exe
2022-09-18 10:04		LAMMPS-ML-PACE-plugin-latest.exe
2022-09-18 10:04		LAMMPS-64bit-Python-latest.exe
2022-09-18 10:04		LAMMPS-64bit-latest.exe
2022-09-18 10:04		LAMMPS-64bit-latest-MPI.exe
2022-09-18 10:00		LAMMPS-USER-VCSGC-plugin-15Sep2022.exe
2022-09-18 10:00		LAMMPS-USER-VCSGC-plugin-15Sep2022-MPI.exe
2022-09-18 10:00		LAMMPS-USER-REBOMOS-plugin-15Sep2022.exe
2022-09-18 10:00		LAMMPS-USER-REBOMOS-plugin-15Sep2022-MPI.exe
2022-09-18 10:00		LAMMPS-USER-AEAM-plugin-15Sep2022.exe
2022-09-18 10:00		LAMMPS-USER-AEAM-plugin-15Sep2022-MPI.exe
2022-09-18 10:00		LAMMPS-ML-PACE-plugin-15Sep2022.exe
2022-09-18 10:00		LAMMPS-USER-AEAM-plugin-15Sep2022-MPI.exe
2022-09-18 10:00		LAMMPS-ML-PACE-plugin-15Sep2022-MPI.exe

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.



The screenshot shows a web browser window at packages.lammps.org/windows.html. The page lists benchmark inputs and reference outputs, and provides instructions for installing MPI support. It mentions that the executables will run in serial when executed directly. The page is titled "MPI Support for LAMMPS on Windows" and explains that users need to install a specific version of MPICH2 from Argonne Lab. It provides instructions for 32-bit and 64-bit Windows, highlighting the latest available binaries: [mpich2-1.4.1p1-win-ia32.msi](#) for 32-bit and [mpich2-1.4.1p1-win-x86-64.msi](#) for 64-bit. A Windows Features dialog box is also shown, with "MPI (x86)" and "MPI (x64)" checked under "Optional Windows features".

MPI Support for LAMMPS on Windows

To use the MPI based parallelism in the provided installer packages, you also need to install a specific version of [MPICH2 from Argonne lab](#). This is a very old version of MPICH for Windows but it is required for these binaries.

For 32-bit Windows you have to download and install [mpich2-1.4.1p1-win-ia32.msi](#). This is the latest available binary 32-bit MPI package compatible with the GNU cross compilers used to compile LAMMPS. Correspondingly, for 64-bit Windows you have to download and install [mpich2-1.4.1p1-win-x86-64.msi](#). This is the latest available binary 64-bit MPI package compatible with the GNU cross compilers used to compile LAMMPS.

For Windows 10 and 11 it may be required to first enable support for .NET 3.5 and older in the Windows settings dialog for optional Windows features of the Control Panel.

There are more recent versions of MPICH ported to Windows by Microsoft, but they are not compatible with the packages here. Also it is not possible to use those packages with the GNU cross-compilers. Instead to use these newer MPI packages you would have to compile LAMMPS from source on Windows yourself using the Microsoft Visual Studio 2022 software. We do not provide precompiled packages created natively on Windows because fewer packages support it and the process of building such packages on Windows has not been sufficiently automated and tested.

Installing LAMMPS globally on Windows with administrator privilege

The installer packages listed above will install LAMMPS into a user's personal storage area and thus it cannot be used by all users. This behavior was changed with the stable release of LAMMPS in October 2020. Installer packages from previous LAMMPS versions and current versions that require administrator privilege to be installed can be found [their own download area](#). The content is otherwise the same, only the packaging is different.

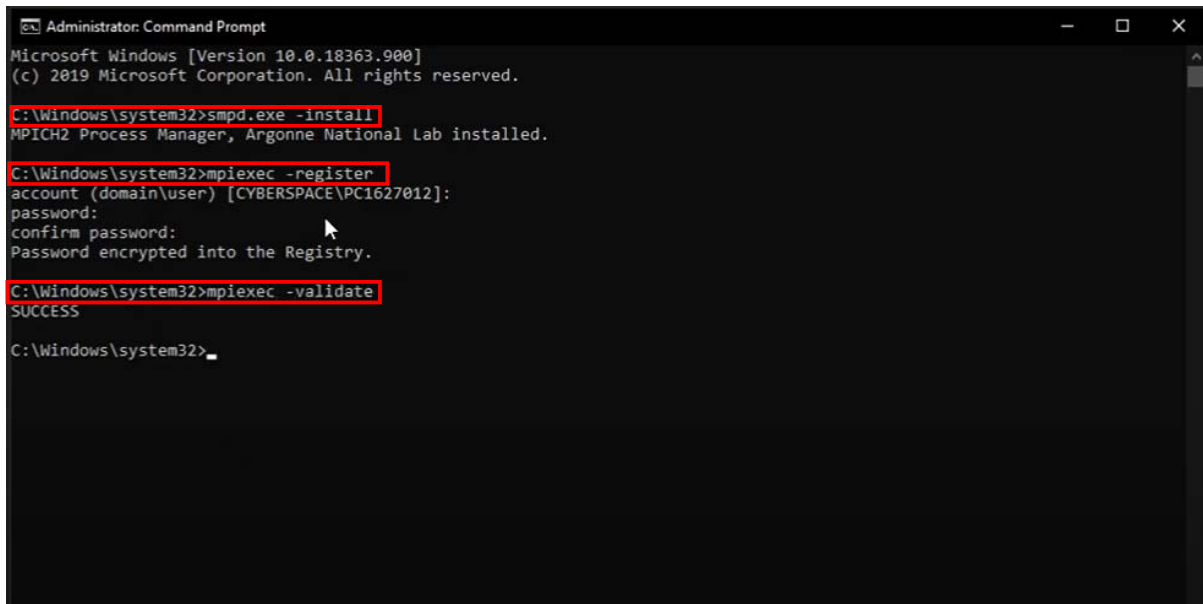
Running LAMMPS on Windows

General Comments

Activate Windows
Go to Settings to activate Windows.

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`



```
Administrator: Command Prompt
Microsoft Windows [Version 10.0.18363.900]
(c) 2019 Microsoft Corporation. All rights reserved.

C:\Windows\system32>smpd.exe -install
MPICH2 Process Manager, Argonne National Lab installed.

C:\Windows\system32>mpiexec -register
account (domain\user) [CYBERSPACE\PC1627012]:
password:
confirm password:
Password encrypted into the Registry.

C:\Windows\system32>mpiexec -validate
SUCCESS

C:\Windows\system32>
```

NOTE: For running LAMMPS-MPI on your system open the folder in which your input and potential files are there then open powershell or terminal 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.

