

Installation guide for LAMMPS on Windows

Feb. 6, 2017

1. Getting LAMMPS

- ① Access to <http://rpm.lammps.org/windows.html>

Visit [\[32-bit Windows download area\]](#) or [\[64-bit Windows download area\]](#).

LAMMPS-ICMS Windows Installer Repository

This repository is hosting pre-compiled Windows installers of the LAMMPS molecular dynamics simulation software package. The binaries are built semi-automatically with MinGW64 Linux to Windows cross compilers using up-to-date snapshots of the [LAMMPS-ICMS git repository](#) hosted at the [Institute for Computational Molecular Science](#) at Temple University. The LAMMPS binaries contain all optional packages included in the source distribution except: KIM (license is not GPL compatible), USER-CUDA (CUDA does not support cross compilation), KOKKOS and USER-INTEL (do not support cross-compilation with GCC), USER-H5MD (requires external library) PYTHON (requires to bundle a full Python runtime), USER-QMMM (only useful when linking to a QM software), USER-QUIP (requires external library), REAX (superseded by the USER-REAXC package which is included). The serial executable additionally does not contain the MPICH and USER-LB packages, since those require MPI-IO functions, which are not available without linking to a real MPI library.

Some Notes on GPU Support

These Windows binaries include (experimental on Windows) GPU acceleration via the GPU package. This is achieved through compiling the GPU package in OpenCL mode and linking to an OpenCL v1.2 compatible ICD loader. This means the executables do not contain any vendor provided code and should be compatible with GPUs from both AMD and Nvidia. The GPU package has been compiled for mixed precision computation and is currently somewhat tuned for Nvidia (Fermi generation) GPUs. It does not yet work with OpenCL drivers for GPUs (like those included in the Intel and AMD OpenCL SDKs).

In the case of having multiple Vendor provided OpenCL runtimes installed, you may run into the situation of the "wrong" runtime being set as the default and used by LAMMPS. In this case, you may need to remove unwanted vendors from the windows registry database. Look for the key: `HKKEY_LOCAL_MACHINE\SOFTWARE\Khronos\OpenCL\Vendors`, and remove vendors such as Intel. When reporting problems, please always include the exact version of the installer, and the output of the `ocl_get_devices` tool.

Looking for pre-compiled Linux binary RPMs? They are just a [mouse click away](#).

Installing LAMMPS on Windows

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

- [Latest version for 32-bit Windows](#) / [32-bit Windows download area](#) for 32-bit versions
- [Latest version for 64-bit Windows](#) / [64-bit Windows download area](#) for 64-bit versions

The respective download directory will contain installer packages that are labeled as `latest`. They were compiled on and one package labeled as `latest`. It is usually recommended to download and install the latest package via the link above. These installer 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:

- A regular multi-threaded LAMMPS executable called `lmp_serial`. This should *always* work.
- A multi-threaded LAMMPS executable that also supports parallel execution via MPI message passing. This executable is called `lmp_mpi` and requires installation of a suitable MPICH2 package to work.
- the LAMMPS manual in PDF format
- the `colvars` reference manual in PDF format
- 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 `restart2data`, `binary2txt`, `chain`, `msilmp`, `ocl_get_devices`

Both executables will run in serial when executed directly. Please see below for instructions on how to use the MPI based parallelism. To use the MPI based parallelism, you also need to install [MPICH2 from Argonne lab](#). For 32-bit Windows you have to download and install [mpich2-1.4.1p1-win-x64-32.msi](#) or any compatible version. Correspondingly, for 64-bit Windows you have to download and install [mpich2-1.4.1p1-win-x64-64.msi](#) or any compatible version.

- ② Download and save `lammps-64bit-20160309.exe` or `lammps-32bit-20160309.exe`. If those versions do not exist, choose the latest one.

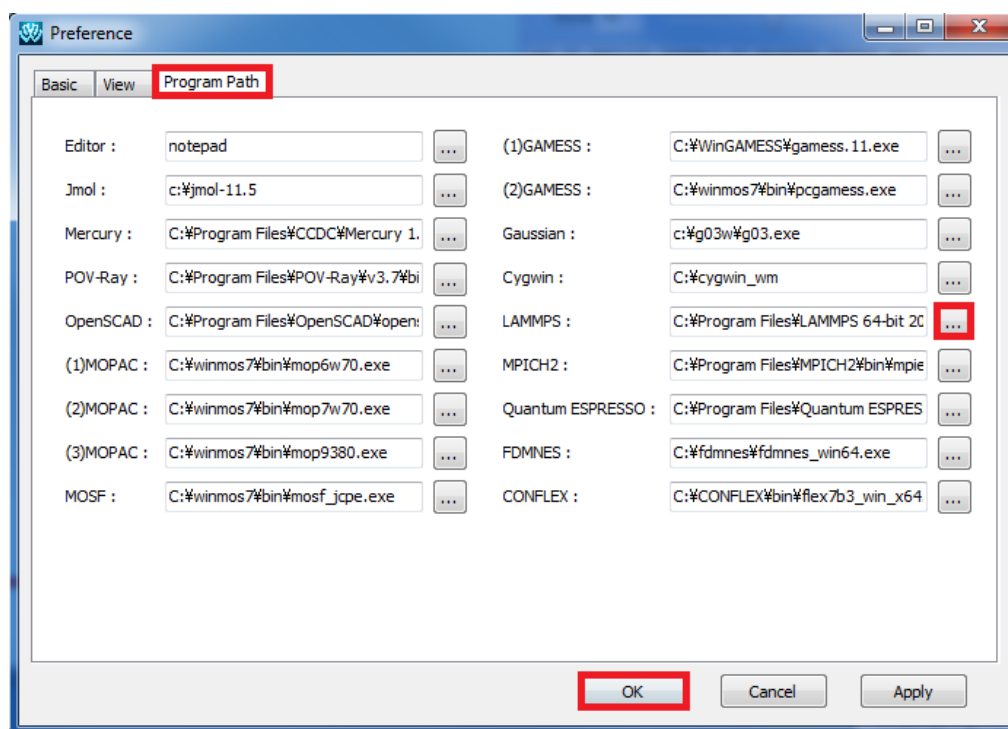
LAMMPS-ICMS Binaries Repository: windows/64bit

Contents of 64bit

[DIR]	(Up one level)
2016-06-08 18:10	lammps-64bit-latest.exe
2016-06-08 18:10	lammps-64bit-20160609.exe
2016-06-03 13:37	lammps-64bit-20160603.exe
2016-05-26 15:31	lammps-64bit-20160526.exe
2016-05-16 13:16	lammps-64bit-20160516.exe
2016-05-11 18:49	lammps-64bit-20160512.exe
2016-05-03 17:04	lammps-64bit-20160503.exe
2016-04-27 16:53	lammps-64bit-20160427.exe
2016-04-19 13:07	lammps-64bit-20160419.exe
2016-04-07 14:30	lammps-64bit-20160407.exe
2016-03-21 10:43	lammps-64bit-20160321.exe
2016-03-08 19:10	lammps-64bit-20160309.exe
2016-02-06 10:28	lammps-64bit-20160206.exe
2015-12-15 12:07	lammps-64bit-20151215.exe

- ③ Double-click the installer file and follow the instructions.

- ④ Launch Winmostar and select [Tools]-> [Preference]. In Preference window, select [Program Path] panel, click [...] button of LAMMPS and choose the executable file. Then, click [OK].



* When lammeps-32bit-20160309.exe has been installed, set to "C:\Program Files\LAMMPS 32-bit 20160309\bin\lmp_serial.exe".

2. Getting cygwin_wm

Access to https://winmostar.com/en/gmx4wm_en.html, download the latest cygwin_wm_*.exe, and follow the instructions. Note that you can skip this step when cygwin_wm has been already installed. Note that you can skip this step when cygwin_wm has been already installed.

3. Getting and setting MPICH

This step is required when parallel executions are needed for LAMMPS.

- ① Access to <http://rpm.lammps.org/windows.html>
- ② Download and save [[mpich2-1.4.1p1-win-x86-64.msi](#)] or [[mpich2-1.4.1p1-win-ia32.msi](#)]. If you use 32-bit version of LAMMPS, choose the latter.
- ③ Double-click the installer file (.msi) and follow the instructions.
- ④ Launch Command Prompt with the administrator authority.
- ⑤ Move to bin in MPICH installation folder.
c:\> cd "c:\Program Files\MPICH2\bin"
- ⑥ Execute the following command.

bin> smpd.exe -install

- ⑦ Launch Winmostar and select [Tools]-> [Preference]. In Preference window, select [Program Path] panel, click [...] button of MPICH2 and choose the executable file mpiexec.exe. Then, click [OK]