

LAMMPS for Windows Installation Manual

April 22, 2020

1. Get LAMMPS

- i. Go to <https://packages.lammps.org/windows.html>. In rare cases, the connection may not work due to server maintenance, etc., but it will be restored in a few days to a week.

※ If it does not recover, download the installer from the following link.

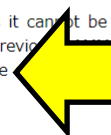
https://winmostar.com/wm/cygvwin_wm/packages/lammps-32bit-20160309.exe

https://winmostar.com/wm/cygvwin_wm/packages/lammps-64bit-20160309.exe

Scroll down to **Installing LAMMPS globally on Windows with administrator privilege** and click on [their own download area].

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 versions and current versions that require administrator privilege to be installed can be found [their own download area](#). The packaging is otherwise the same, only the packaging is different.

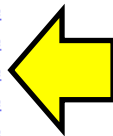


- ii. Click directory link of [64bit] or [32bit] and save lammps-64bit-20160309.exe for 64bit or lammps-32bit-20160309.exe for 32bit.

LAMMPS-ICMS Binaries Repository: windows/64bit

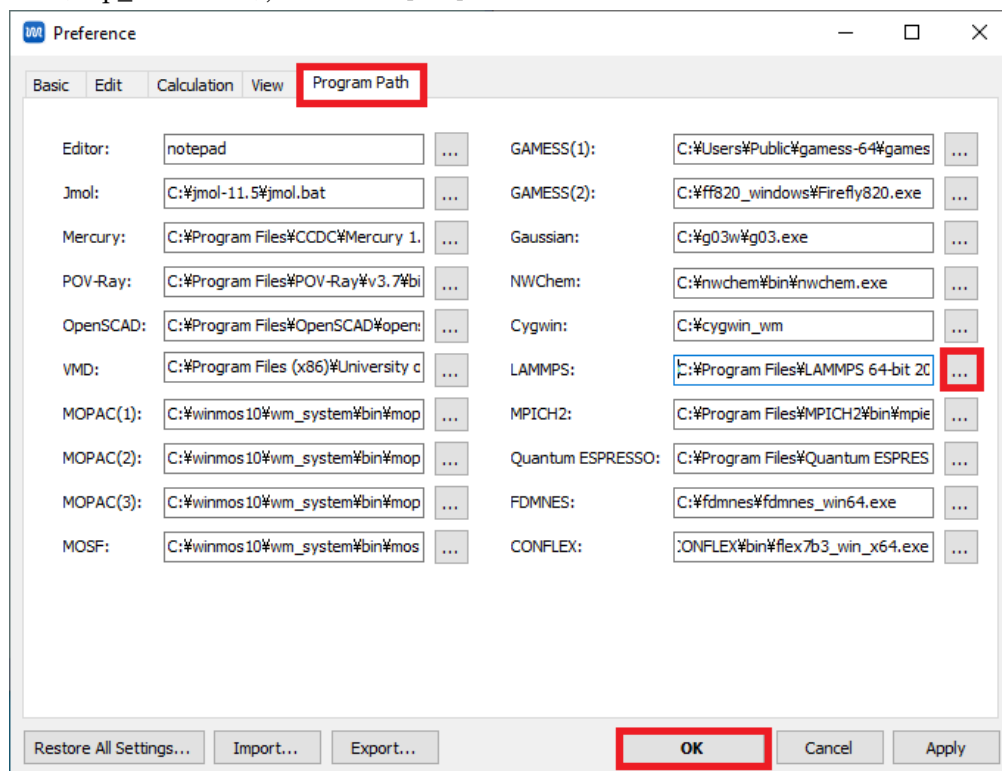
Contents of 64bit

[DIR]	(Up one level)
2016-05-04 12:43	lammps-64bit-latest.exe
2016-05-04 12:43	lammps-64bit-20160504.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
2016-02-28 12:20	lammps-64bit-20160228.exe
2016-02-16 08:36	lammps-64bit-20160216.exe
2016-02-06 10:28	lammps-64bit-20160206.exe



- iii. Double-click the saved exe file and follow the instructions.
- iv. To set the path for Winmostar to call LAMMPS, click [Tools] → [Preferences] in Winmostar to open the Preference panel. Open the [Program Path] tab of the Preference Panel, and click the [...] button of [LAMMPS] to register the LAMMPS executable file (lmp_serial.exe). Register the LAMMPS executable

file (lmp_serial.exe), and click [OK].

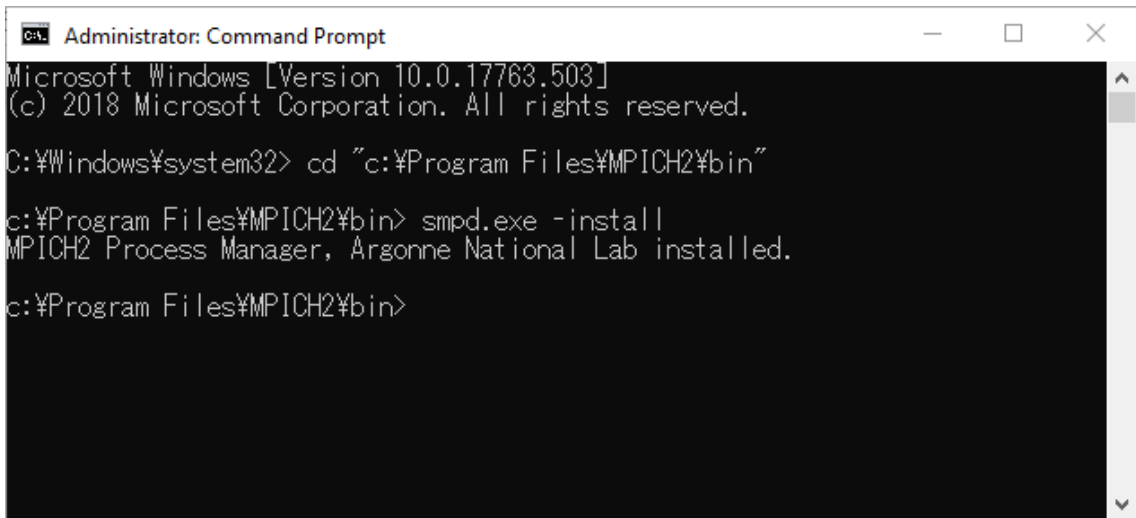


※By default, it is displayed as

C:\Program Files\LAMMPS 64-bit 20160309\bin\lmp_serial.exe. If you want to use 32bit one, change it to C:\Program Files\LAMMPS 32-bit 20160309\bin\lmp_serial.exe, etc.

2. Obtain and set up cygwin_wm (not necessary if cygwin_wm has already been set up)
Download the cygwin_wm installer from the following link and set up.
https://winmostar.com/en/gmx4wm_en.html
3. Obtain and install MPICH (required only if you want to run LAMMPS in parallel)
 - i. Click [[mpich2-1.4.1p1-win-ia32.msi](#)] or [[mpich2-1.4.1p1-win-x86-64.msi](#)] to download the MSI file (if the extension is changed, revert to .msi), depending on the OS. If LAMMPS is 32-bit, select 32-bit MPICH (if it is 64-bit, select 64-bit).
 - ii. Double-click on the saved MSI file and follow the instructions. If the installation fails, download .NET Framework 3.5 from <https://www.microsoft.com/en-US/download/details.aspx?id=21>. Windows 8.1/10 comes with .NET Framework 4.5 by default, but you need to install 3.5 separately.
 - iii. Start a command prompt from the start menu with administrative privileges.
 - iv. Go to the folder where you installed MPICH.
C:\> cd "C:\Program Files\MPICH2\bin"
 - v. Execute the MPICH setup command (smpd.exe).

C:\Program Files\MPICH2\bin> smpd.exe -install



```
Administrator: Command Prompt
Microsoft Windows [Version 10.0.17763.503]
(c) 2018 Microsoft Corporation. All rights reserved.

C:\Windows\system32> cd "c:\Program Files\MPICH2\bin"

c:\Program Files\MPICH2\bin> smpd.exe -install
MPICH2 Process Manager, Argonne National Lab installed.

c:\Program Files\MPICH2\bin>
```

- vi. (6) Click [Tools] → [Preferences] in Winmostar to open the Preference panel. Open the [Program Path] tab in the Preference Panel, and click the [...] button for [MPICH2]. Register the MPICH executable file (mpiexec.exe) and click [OK].

4. Obtain and install potential files for inorganic compounds (if necessary)
 - i. Go to the website [NIST Interatomic Potentials Repository](https://www.nist.gov/patents/interatomic-potentials-repository), and click an element of you want to calculate.

Interatomic Potentials (Force Fields)

Elements

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu	86 Rn
87 Fr	88 Ra	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr	112 Og

- ii. Search the term including all elements you want to calculate.

Al-Ni

2015--Kumar-A-Chernatynskiy-A-Liang-T-et-al--Al-Ni

Citation: A. Kumar, A. Chernatynskiy, T. Liang, K. Choudhary, M.J. Noordhoek, Y.-T. Cheng, S.R. Phillpot, and S.B. Sinnott (2015), "Charge optimized many-body (COMB) potential for dynamical simulation of Ni-Al phases", *Journal of Physics: Condensed Matter*, **27(33)**, 336302. DOI: [10.1088/0953-8954/27/33/336302](https://doi.org/10.1088/0953-8954/27/33/336302).

Abstract: An interatomic potential for the Ni-Al system is presented within the third-generation charge optimized many-body (COMB3) formalism. The potential has been optimized for Ni₃Al, or the γ' phase in Ni-based superalloys. The formation energies predicted for other Ni-Al phases are in reasonable agreement with first-principles results. The potential further predicts good mechanical properties for Ni₃Al, which includes the values of the complex stacking fault (CSF) and the anti-phase boundary (APB) energies for the (1 1 1) and (1 0 0) planes. It is also used to investigate dislocation propagation across the Ni₃Al (1 1 0)-Ni (1 1 0) interface, and the results are consistent with simulation results reported in the literature. The potential is further used in combination with a recent COMB3 potential for Al₂O₃ to investigate the Ni₃Al (1 1 1)-Al₂O₃ (0 0 0 1) interface, which has not been modeled previously at the classical atomic level due to the lack of a reactive potential to describe both Ni₃Al and Al₂O₃ as well as interactions between them. The calculated work of adhesion for this interface is predicted to be 1.85 J m⁻², which is in agreement with available experimental data. The predicted interlayer distance is further consistent with the available first-principles results for Ni (1 1 1)-Al₂O₃ (0 0 0 1).

LAMMPS pair_style comb3 (2015--kumar-a--al-ni--lammps-mp1)

See Computed Properties

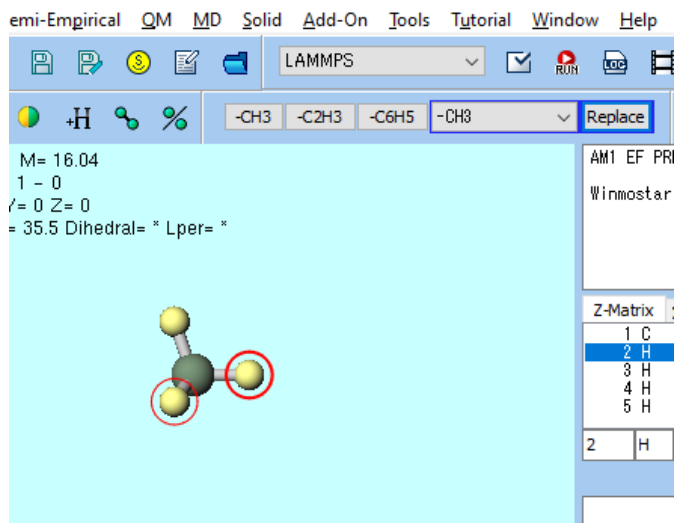
Notes: This file was obtained from Jarvis-FF (<https://www.ctcms.nist.gov/~knc6/periodic.html>) on 9 Nov. 2018 and posted at Kamal Choudhary's (NIST) request.

File(s):
ffield.comb3.NiAlO

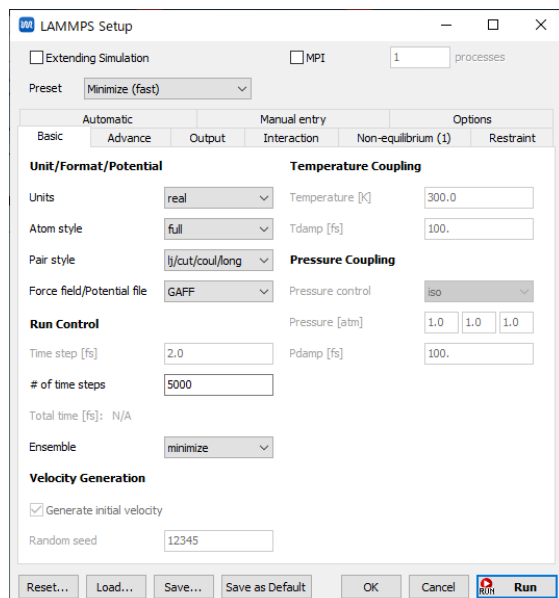
- iii. Right-click the link of "Files(s):", and save the file.
- iv. Copy the downloaded file to the Potentials folder in your LAMMPS installation folder (default: C:\Program Files\LAMMPS 64-bit 20160309\Potentials).

5. Simple operation check

- i. Click [File]-[New] in the main menu of Winmostar, and then click [Replace] button at the upper center of the main window to create a methane molecule.

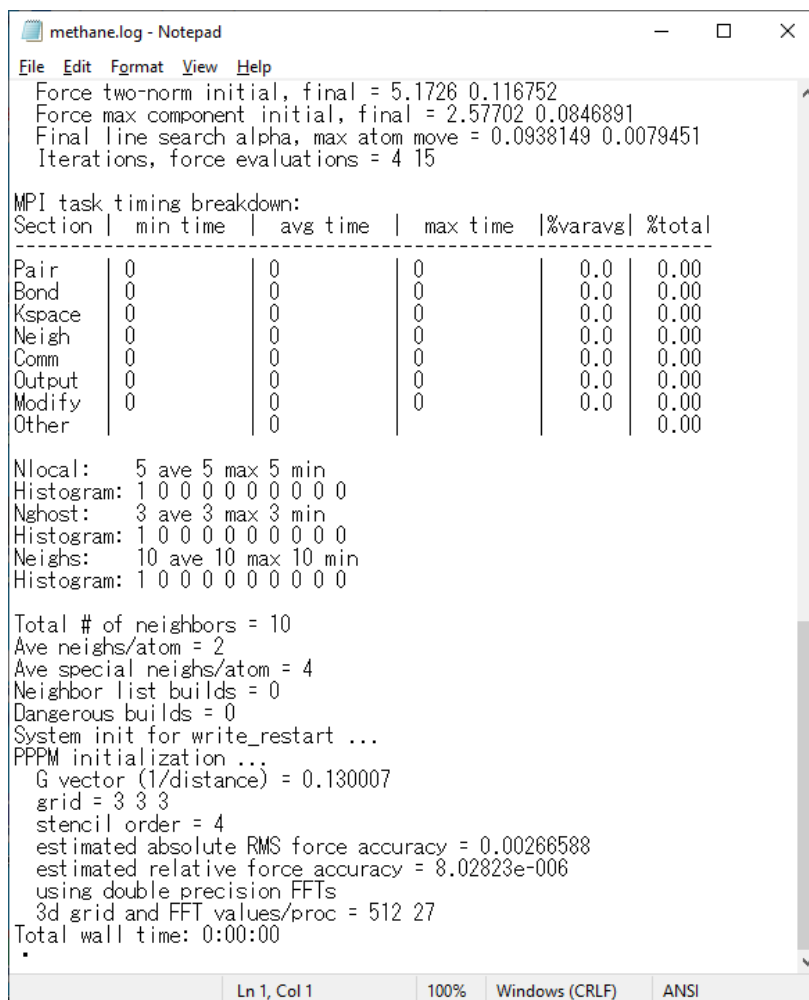


- ii. Click on [MD]-[LAMMPS]-[Configure] and you'll see "Some molecules do not have charges. Do you want to assign charges now?" In the dialog box, press [Yes] button.
- iii. A dialog box with "Assign charges" will appear. Press [OK] with the default value.
- iv. A dialog box with "Create Cell" will appear. Press [OK] with the default value.
- v. A dialog box with "Assign force field parameters" will appear. Press [OK] button with the default value.
- vi. Click the [Run] button at the bottom right of the LAMMPS Setup window.



- vii. A save dialog opens, and when you save it with a suitable name, a black terminal window opens and a lot of messages flow. After a while, the process is over and the terminal window closes.

- viii. Click [MD]-[LAMMPS]-[Open Log File (log)] and open the file selected by default in the dialog. When the LAMMPS calculation succeeded, you will see the statistics of the calculation at the end of the opened text file.



```
methane.log - Notepad
File Edit Format View Help
Force two-norm initial, final = 5.1726 0.116752
Force max component initial, final = 2.57702 0.0846891
Final line search alpha, max atom move = 0.0933149 0.0079451
Iterations, force evaluations = 4 15

MPI task timing breakdown:
Section | min time | avg time | max time | %varavg | %total
-----|-----|-----|-----|-----|-----
Pair    | 0         | 0         | 0         | 0.0      | 0.00
Bond    | 0         | 0         | 0         | 0.0      | 0.00
Kspace  | 0         | 0         | 0         | 0.0      | 0.00
Neigh   | 0         | 0         | 0         | 0.0      | 0.00
Comm    | 0         | 0         | 0         | 0.0      | 0.00
Output  | 0         | 0         | 0         | 0.0      | 0.00
Modify  | 0         | 0         | 0         | 0.0      | 0.00
Other   | 0         | 0         | 0         | 0.0      | 0.00

Nlocal: 5 ave 5 max 5 min
Histogram: 1 0 0 0 0 0 0 0 0
Nghost: 3 ave 3 max 3 min
Histogram: 1 0 0 0 0 0 0 0 0
Neighs: 10 ave 10 max 10 min
Histogram: 1 0 0 0 0 0 0 0 0

Total # of neighbors = 10
Ave neighs/atom = 2
Ave special neighs/atom = 4
Neighbor list builds = 0
Dangerous builds = 0
System init for write_restart ...
PPPM initialization ...
G vector (1/distance) = 0.130007
grid = 3 3 3
stencil order = 4
estimated absolute RMS force accuracy = 0.00266588
estimated relative force accuracy = 8.02823e-006
using double precision FFTs
3d grid and FFT values/proc = 512 27
Total wall time: 0:00:00
.
```