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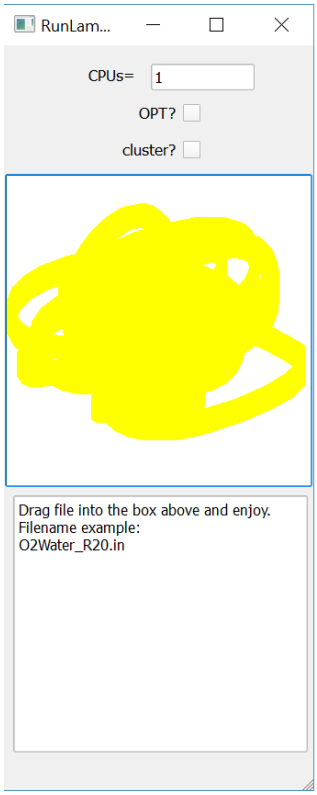
How to run lammps simulation using only 1 core (serial run)?

1. Build a new subfolder in this folder, e.g. "Jobs2". Make sure there is no "space" in the folder name. For example, a subfolder named "Project 1" is not good.

2. Double click "RunLAMMPSMulti.exe" in this folder, and a window will pop up like this,



3. Drag the input file (e.g. tensile.in located in the Jobs2 folder) into the box highlighted in the above figure.

4. Enjoy the simulation!

Caution:

The Lammps executable is located in the "Bin" folder.

In general, two files are needed to run the lammps simulation,

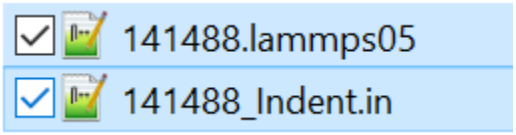
1) Geometry file (*.lammps05), containing the information about the location and type of atoms in the system.
2) Input file (*.in), containing the information about the force field, loading, constraints and the temporal evolution of the system.

For the above procedure (drap and drop to run lammps) to work properly. A strict naming rule should be followed,

Geometry file should be named as *.lammps05. No “_” is allowed in the name.

Input file should be named as X_Y.lammps, where X is the name of the geometry file. No “_” is allowed in Y.

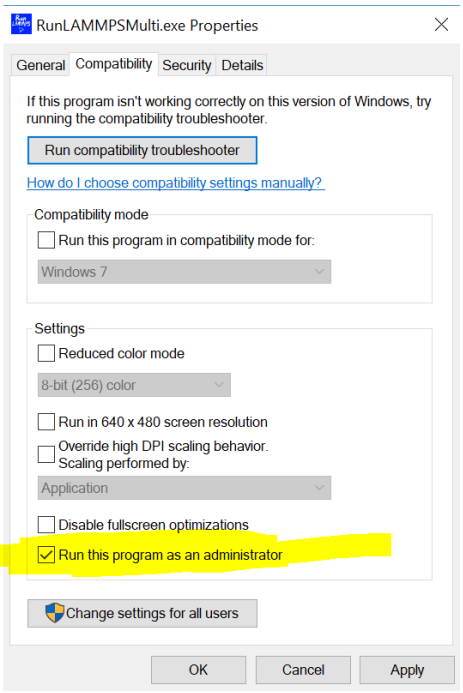
For example:



When you would like to run lammps, drag the 141488_Indent.in to the window. And that is it.

How to run lammps simulation using n cores (parallel run)?

0. Right click the mpiexec.exe in “Bin” folder and select properties. Then choose “Run this program as an administrator” on the Compatibility tab, as shown below:



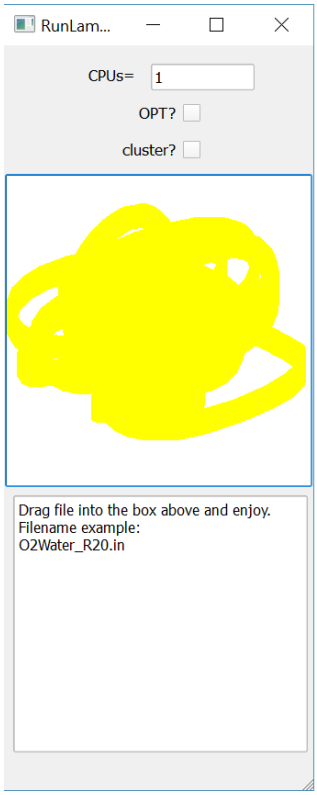
You only need to do this once.

Then install the MPICH2 by running LAMMPS/mpich2/mpich2-1.4.1p1-win-x86-64.exe.

After you installed MPICH2, run SERVICES.MSC to check if there is a service called “MPICH2”. If not, open cmd with admin rights and “cd” into the mpich2 folder. Then run the command: smpd -install.

1. Build a new subfolder in this folder, e.g. "Jobs2". Make sure there is no "space" in the folder name. For example, a subfolder named "Project 1" is not good.

2. Double click "RunLAMMPSMulti.exe" in this folder, a window will pop up like this,



3. Set the number of cores you will use as n. Then drag the input file (e.g. tensile.in located in the Jobs2 folder) into the box highlighted in the above figure.

4. Enjoy the simulation!