

8.6.3 Using the LAMMPS GUI

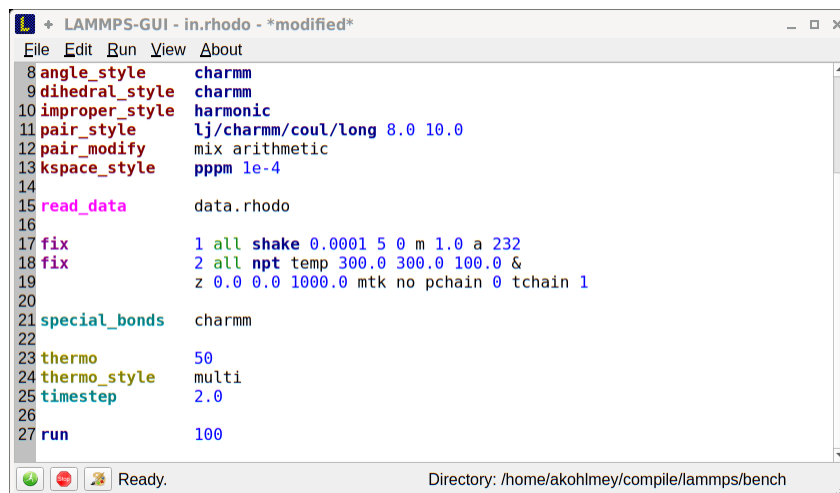
LAMMPS GUI is a simple graphical text editor that is linked to the *LAMMPS C-library interface* and thus can run LAMMPS directly using the contents of the editor's text buffer as input.

This is similar to what people traditionally would do to run LAMMPS: using a regular text editor to edit the input and run the necessary commands, possibly including the text editor, too, from a command line terminal window. That is quite effective when running LAMMPS on high-performance computing facilities and when you are very proficient in using the command line. The main benefit of a GUI application is that this integrates well with graphical desktop environments and many basic tasks can be done directly from within the GUI without switching to a text console or requiring external programs or scripts to extract data from the generated output. This makes it easier for beginners to get started running simple LAMMPS simulations and thus very suitable for tutorials on LAMMPS. But also makes it easier to switch to a full featured text editor and more sophisticated visualization and analysis tools.

The following text provides a detailed tour of the features and functionality of the LAMMPS GUI. This document describes LAMMPS GUI version 1.2.

Main window

When LAMMPS GUI starts, it will show the main window with either an empty buffer, or have a file loaded. In the latter case it may look like the following:



```

LAMMPS-GUI - in.rhodo - *modified*
File Edit Run View About
8 angle_style charmm
9 dihedral_style charmm
10 improper_style harmonic
11 pair_style lj/charmm/coul/long 8.0 10.0
12 pair_modify mix arithmetic
13 kspace_style pppm 1e-4
14
15 read_data data.rhodo
16
17 fix 1 all shake 0.0001 5 0 m 1.0 a 232
18 fix 2 all npt temp 300.0 300.0 100.0 &
19 z 0.0 0.0 1000.0 mtk no pchain 0 tchain 1
20
21 special_bonds charmm
22
23 thermo 50
24 thermo_style multi
25 timestep 2.0
26
27 run 100
  
```

Ready. Directory: /home/akohlmei/compile/lammps/bench

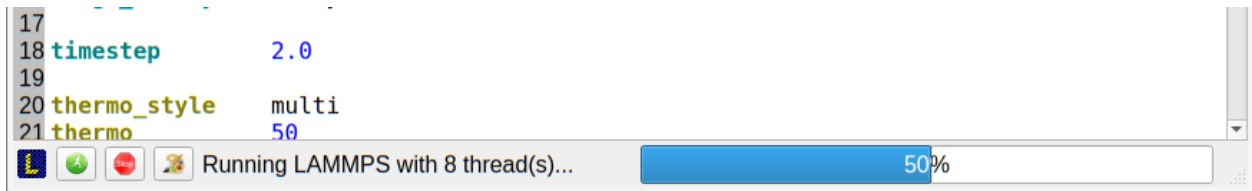
There is the menu bar at the top, then the main editor buffer with the input file contents in the center with line numbers on the left and the input colored according to the LAMMPS input file syntax. At the bottom is the status bar, which shows the status of LAMMPS execution on the left (“Ready.” when idle) and the current working directory on the right. The size of the main window will be stored when exiting and restored when starting again. The name of the current file in the buffer is shown in the window title and the text **modified** is added in case the buffer has modifications that are not yet saved to a file.

Opening Files

The LAMMPS GUI application will try to open the first command line argument as input file, further arguments are ignored. When no argument is given LAMMPS GUI will start with an empty buffer. Files can also be opened via the File menu or by drag-and-drop of a file from a file manager to the editor window. Only one file can be open at a time, so opening a new file with a filled buffer will close this buffer and in case the buffer has unsaved modifications will ask to either cancel the load, discard the changes or save them.

Running LAMMPS

From within the LAMMPS GUI main window LAMMPS can be started either from the Run menu, by the hotkey *Ctrl-Enter* (*Command-Enter* on macOS), or by clicking on the green button in the status bar. LAMMPS runs in a separate thread, so the GUI stays responsive and thus it is able to interact with the calculation and access its data. It is important to note, that LAMMPS is using the contents of the input buffer for the run, **not** the file it was read from. If there are unsaved changes in the buffer, they *will* be used.

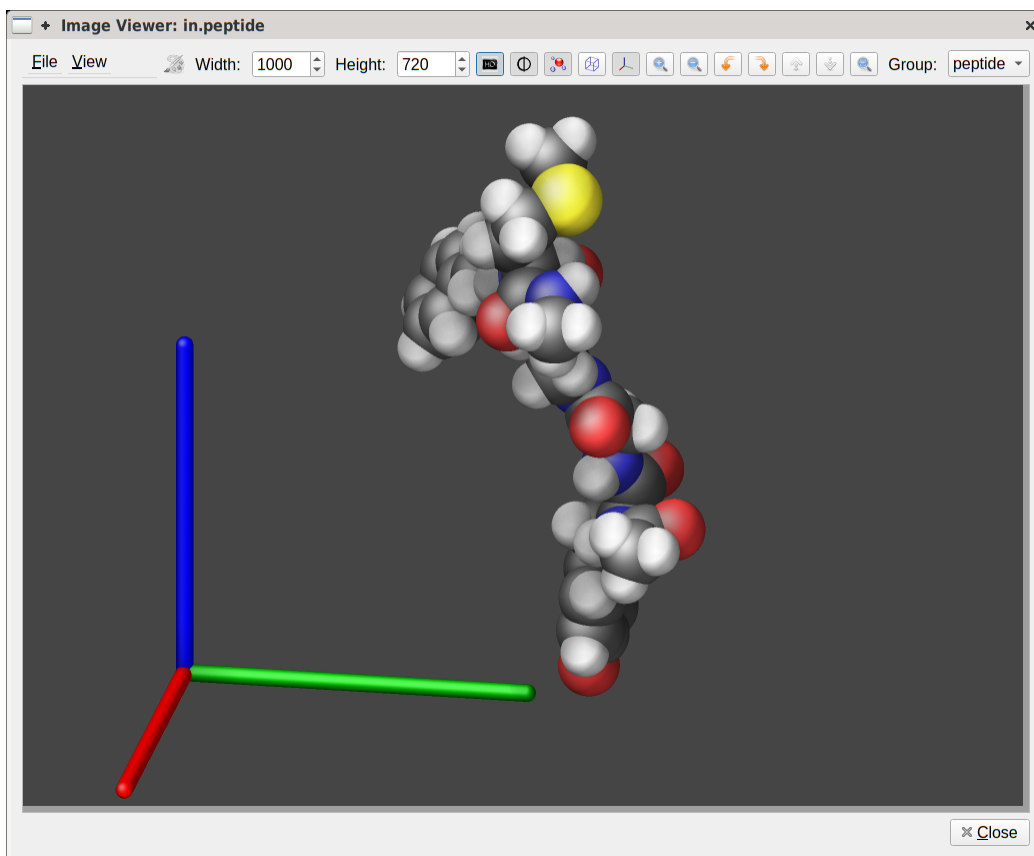


While LAMMPS is running, the contents of the status bar change: on the left side there is a text indicating that LAMMPS is running, which will contain the selected number of threads, if thread-parallel acceleration was selected in the Preferences dialog. On the right side, a progress bar is shown that displays the estimated progress on the current *run command*. Additionally, two windows will open: the log window with the captured screen output and the chart window with a line graph created from the thermodynamic output of the run.

The run can be stopped cleanly by using either the Stop LAMMPS entry in the Run menu, the hotkey *Ctrl-/* (*Command-/* on macOS), or clicking on the red button in the status bar. This will cause that the running LAMMPS process will complete the current iteration and then stop. This is equivalent to the command *timer timeout 0 <timer>* and implemented by calling the `lammops_force_timeout()` function of the LAMMPS C-library interface.

Viewing Snapshot Images

By selecting the View Image entry in the Run menu, by hitting the *Ctrl-I* (*Command-I* on macOS) hotkey or by clicking on the “palette” button in the status bar, LAMMPS GUI will issue a `write_dump image` command and read the resulting snapshot image into an image viewer window. When possible, LAMMPS GUI will try to detect which elements the atoms correspond to (via their mass) and then colorize them accordingly. Otherwise just some predefined sequence of colors are assigned to different atom types.



The default image size, some default image quality settings, the view style and some colors can be changed in the Preferences dialog window. From the image viewer window further adjustments can be made: actual image size, high-quality rendering, anti-aliasing, view style, display of box or axes, zoom factor. The image can be rotated horizontally and vertically and it is possible to only display the atoms within a predefined group (default is “all”). After each change, the image is rendered again and the display updated. The small palette icon on the top left will be colored while LAMMPS is running to render the image and it will be grayed out again, when it is done. When there are many items to show and high quality images with anti-aliasing are requested, re-rendering can take several seconds. From the File menu, the shown image can be saved to a file permanently or copied into the cut-n-paste buffer for pasting into another application.

Editor Functions

The editor has most the usual functionality that similar programs have: text selection via mouse or with cursor moves while holding the Shift key, Cut, Copy, Paste, Undo, Redo. All of these editing functions are available via hotkeys. When trying to exit the editor with a modified buffer, a dialog will pop up asking whether to cancel the quit, or don't save or save the buffer's contents to a file.

Context Specific Help



A unique feature of the LAMMPS GUI is the option to look up the documentation for the command in the current line. This can be achieved by either clicking the right mouse button or by using the *Ctrl-?* hotkey. When clicking the mouse there are additional entries in the context menu that will open the corresponding documentation page in the online LAMMPS documentation. When using the hotkey, the first of those entries will be chosen directly.

Menu

The menu bar the entries File, Edit, Run, View, and About. Instead of using the mouse to click on them, the individual menus can also be activated by hitting the *Alt* key together with the corresponding underlined letter, that is *Alt-f* will activate the File menu. For the corresponding activated sub-menus, also the underlined letter, together with the *Alt* key can be used to select instead of the mouse.

File

The File menu offers the usual options:

- New will clear the current buffer and reset the file name to **unknown**
- Open will open a dialog to select a new file
- Save will save the current file; if the file name is **unknown** a dialog will open to select a new file name
- Save As will open a dialog to select and new file name and save the buffer to it
- Quit will exit LAMMPS GUI. If there are unsaved changes, a dialog will appear to either cancel the quit, save or don't save the file.

In addition, up to 5 recent file names will be listed after the Open entry that allows to re-open recent files. This list is stored when quitting and recovered when starting again.

Edit

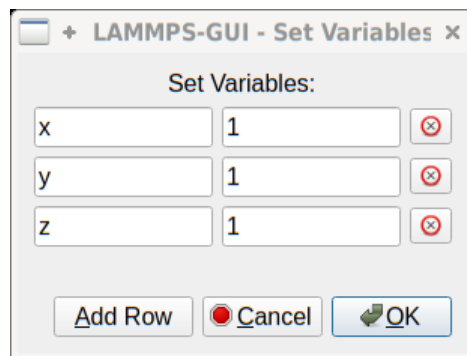
The Edit menu offers the usual editor functions like Undo, Redo, Cut, Copy, Paste, but also offers to open the Preferences dialog and to delete all stored preferences so they will be reset to their defaults.

Run

The Run menu allows to start and stop a LAMMPS process. Rather than calling the LAMMPS executable as a separate executable, the LAMMPS GUI is linked to the LAMMPS library and thus can run LAMMPS internally through the *LAMMPS C-library interface*. Specifically, a LAMMPS instance will be created by calling `lammips_open_no_mpi()` and then the buffer contents run by calling `lammips_commands_string()`. Certain commands and features are only available, after a LAMMPS instance is created. Its presence is indicated by a small LAMMPS L logo in the status bar at the bottom left of the main window.

The LAMMPS calculation will be run in a concurrent thread so that the GUI will stay responsive and will be updated during the run. This can be used to tell the running LAMMPS instance to stop at the next timestep. The Stop LAMMPS entry will do this by calling `lammips_force_timeout()`, which is equivalent to a `timer timeout 0` command.

The Set Variables entry will open a dialog box where *index style variables* can be set. Those variables will be passed to the LAMMPS instance when it is created and are thus set *before* a run is started.



The Set Variables dialog will be pre-populated with entries that are set as index variables in the input and any variables that are used but not defined as far as the built-in parser can detect them. New rows for additional variables can be added through the Add Row button and existing rows deleted by clicking on the X icons on the right.

The View Image entry will send a `dump image` command to the LAMMPS instance, read the resulting file, and show it in an Image Viewer window.

The View in OVITO entry will launch OVITO with a *data file* of the current state of the system. This option is only available, if the LAMMPS GUI can find the OVITO executable in the system path.

The View in VMD entry will instead launch VMD, also to load a *data file* of the current state of the system. This option is only available, if the LAMMPS GUI can find the VMD executable in the system path.

View

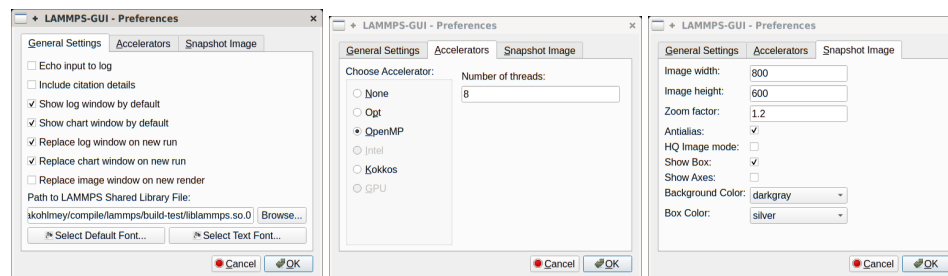
The View menu offers to show or hide the three optional windows with log output, graphs, or images. The default settings for those can be changed in the Preferences dialog.

About

The About menu finally offers a couple of dialog windows and an option to launch the LAMMPS online documentation in a web browser. The About LAMMPS GUI entry displays a dialog with a summary of the configuration settings of the LAMMPS library in use and the version number of LAMMPS GUI itself. The Quick Help displays a dialog with a minimal description of LAMMPS GUI. And LAMMPS Manual will open the main page of this LAMMPS documentation at <https://docs.lammps.org/>.

Preferences

The Preferences dialog allows to customize some of the behavior and looks of the LAMMPS GUI application. The settings are grouped and each group is displayed within a tab.



General Settings:

- *Echo input to log:* when checked, all input commands, including variable expansions, will be echoed to the log window. This is equivalent to using `-echo screen` at the command line. There is no log file produced since it always uses `-log none`.
- *Include citation details:* when checked full citation info will be included to the log window. This is equivalent to using `-cite screen` on the command line.
- *Show log window by default:* when checked, the screen output of a LAMMPS run will be collected in a log window during the run
- *Show chart window by default:* when checked, the thermodynamic output of a LAMMPS run will be collected and displayed in a chart window as line graphs.
- *Replace log window on new run:* when checked, an existing log window will be replaced on a new LAMMPS run, otherwise each run will create a new log window.
- *Replace chart window on new run:* when checked, an existing chart window will be replaced on a new LAMMPS run, otherwise each run will create a new chart window.
- *Replace image window on new render:* when checked, an existing chart window will be replaced when a new snapshot image is requested, otherwise each command will create a new image window.
- *Path to LAMMPS Shared Library File:* this options is only available when LAMMPS GUI was compiled to load the LAMMPS library at run time instead of being linked to it directly. With the `Browse...` button or by changing

the text, a different shared library file with a different compilation of LAMMPS with different settings or from a different version can be loaded. After this setting was changed, LAMMPS GUI needs to be re-launched.

- *Select Default Font*: Opens a font selection dialog where the type and size for the default font (used for everything but the editor and log) of the application can be set.
- *Select Text Font*: Opens a font selection dialog where the type and size for the text editor and log font of the application can be set.

Accelerators:

This tab enables to select which accelerator package is used and is equivalent to using the *-suffix* and *-package* flags on the command line. Only settings supported by the LAMMPS library and local hardware are available. The *Number of threads* field allows to set the maximum number of threads for the accelerator packages that use threads.

Snapshot Image:

This tab allows to set some defaults for the snapshot images displayed in the `Image Viewer` window, like its dimensions and the zoom factor applied. The *Antialias* switch requests to render images with twice the number of pixels for width and height and then smoothly scales the image back to the requested size. This produces higher quality images with smoother edges at the expense of requiring more CPU time to render the image. The *HQ Image mode* option turns on using a screen space ambient occlusion mode (SSAO) when rendering images. This is also more time consuming, but produces a more ‘spatial’ representation of the system. The *VDW Style* checkbox selects whether atoms are represented by space filling spheres when checked or by smaller spheres and stick. Finally there are a couple of drop down lists to select the background and box color.

Hotkeys

Almost all functionality is accessible from the menu or via hotkeys. The following hotkeys are available (On macOS use the Command key instead of Ctrl/Control).

Hotkey	Function	Hotkey	Function	Hotkey	Function	Hotkey	Function
Ctrl+N	New File	Ctrl+Z	Undo edit	Ctrl+Enter	Run LAMMPS	Ctrl+Shift+L	About LAMMPS GUI
Ctrl+O	Open File	Ctrl+Shift+Z	Redo edit	Ctrl+/	Stop Active Run	Ctrl+Shift+H	Quick Help
CTRL+S	Save File	Ctrl+C	Copy text	Ctrl+Shift+V	Set Variables	Ctrl+Shift+G	LAMMPS GUI Howto
Ctrl+Shift+S	Save File As	Ctrl+X	Cut text	Ctrl+I	Create Snapshot Image	Ctrl+Shift+M	LAMMPS Manual
Ctrl+Q	Quit	Ctrl+V	Paste text	Ctrl+P	Preferences	Ctrl+?	Context Help

Further editing keybindings are documented with the [Qt documentation](#). In case of conflicts the list above takes precedence.