Moltemplate Manual

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Contents

Warning: This manual does not explain how build molecules that use all-atom force fields, or how to to run reactive (a.k.a. "active-matter") simulations.

However numerous examples and README files are available to demonstrate how to run these kinds of simulations. Downloading these examples is highly recommended. (See section 2.)

1 Introduction

Moltemplate is a general molecule builder and force-field database system for LAMMPS. A simple file format has been created to store molecule definitions and force-fields (the LAMMPS-template format, LT). LT files are templates containing *all* of the text relevant to a particular molecule (including coordinates, bond-topology, angles, force-field parameters, constraints, groups and fixes). Moltemplate can then duplicate the molecule, customize it, and use it as a building-block for constructing larger, more complex molecules. (These molecules can be used to build larger molecules.) Once built, individual molecules and subunits can be customized (atoms and bonds, and subunits can be inserted, moved, deleted and/or replaced).

Moltemplate is extremely flexible. It supports all LAMMPS force-field styles and nearly all atom-styles (now and in the future).

All-atom simulations

Moltemplate was designed for coarse-grained simulations. To prepare realistic all-atom simulations, you can *either* use the **ATB** service (`https://atb.uq.edu.au`) to download a realistic LT file describing your molecules, *or* create an LT file by hand. In the later case, if you want to use one of the force-field parameter sets included with moltemplate (eg. OPLSAA, GAFF2, COMPASS), you must choose the *type* of each atom in the molecule by hand. ***Moltemplate does not assign atom types automatically.*** For example, to create an LT file for a molecule that contains a carbon atom, you must choose which *type* of carbon atom is most appropriate for that atom. (For most force fields, there are many types of carbon atoms to choose from.) To do that, you must choose a force field (eg. OPLSAA), and read the force field's LT file (eg. "oplsaa.lt"), and choose from the list of atom type descriptions in that file, the one which most closely matches that atom. (Its partial charge may also need to be adjusted.) This is not difficult for simple organic molecules like polyethylene or benzene, but it is not trivial for complex molecules like proteins and many ligands.

Unlike other molecule builders, moltemplate does not infer atom types from their local bond environment or from information from PDB files. Moltemplate also does not repair incomplete PDB files or calculate atomic partial charges using physics. While moltemplate can read PDB files, ***moltemplate currently only reads atomic coordinates from PDB files and discards all other information.***

Strategy for preparing all atom simulations

Consequently, for complex molecules, users are currently encouraged to either use **ATB** [1], *or* prepare simulation files using a different molecule building program that supports automatic atom type (and charge) assignment, and save (or convert) the resulting files to LAMMPS DATA format. Once in LAMMPS DATA format, they can be converted into moltemplate format (if desired) using the "ltemplify.py" utility. (See appendix B.)

Requirements

Moltemplate requires the Bourne-shell, and a recent version of python (2.7 or 3.0 or higher), and can run on OS X, linux, or windows (if a suitable shell environment has been installed). **A substantial amount of memory is needed** to run moltemplate. For example, building a system of 1000000 atoms typically requires between 3 and 12 GB of *available* memory. (This depends on the number of bonds, molecules, and angular interactions. See section 11 for details.)

1.1 Converting *LT files* to LAMMPS input/data files

The moltemplate.sh program converts LT-files (which contain molecule definitions) into complete LAMMPS input-scripts and data-files:

```
moltemplate.sh -atomstyle "full" system.lt
```

or

```
moltemplate.sh -xyz coords.xyz -atomstyle "full" -vmd system.lt
```

In the first example, the coordinates of the atoms in the system are built from commands inside the "system.lt" file. In the second example coordinates for the atoms are read from an XYZ-file, and then VMD is invoked to visualize the system just created. (PDB-files and other coordinate formats are also supported. Note: The "full" atom style was used in this example, but other LAMMPS atom styles are supported, including hybrid styles.)

Either of these commands will construct a LAMMPS data file and a LAMMPS input script (and possibly one or more auxiliary input files), which can be directly run in LAMMPS with minimal editing.

1.2 Converting LAMMPS input/data files to *LT files*

Existing LAMMPS input/data files can be converted into ".LT" files using the "ltemplify.py" utility. (*Some additional manual editing may be required. See appendix B.*)

Additional tools

The **ATB** service [1] mentioned earlier (`https://atb.uq.edu.au`) is a repository of hundreds of thousands of carefully parameterized molecules. Users can submit requests for molecules which are not yet in the repository. Both the charge and force-field parameters for these molecules have been individually optimized using quantum chemical calculations. These molecules are available in moltemplate's native "LT" format.

Moltemplate can also read LAMMPS DATA files files generated by other tools, including VMD/topotools [2] and OpenBabel [3]. These data files can be converted into "LT" format using the "ltemplify.py" utility. VMD [4], topotools [2], and OVITO [5] are also useful for visualizing the data files and trajectory files created by moltemplate.sh and LAMMPS. (See section 4.3.)

The PACKMOL [6] program is useful for generating coordinates of dense heterogeneous mixtures of molecules, which can be read by moltemplate. (The VMD "solvate" plugin may also be helpful.)

Examples

This manual explains in detail how to use moltemplate.sh to build LAMMPS files from scratch. You will also need to learn how to *run* LAMMPS and visualize your results. Section 4 contains a brief tutorial which explains how to build a box of water using moltemplate and visualize initial conformation, run LAMMPS, and then visualize the trajectory. Several complete working examples (with images and readme files) which can be downloaded and modified are available online at: `http://moltemplate.org/visual_examples.html` A more comprehensive list of examples is included in the "examples/" subdirectory distributed with moltemplate. These examples are a good starting point for learning LAMMPS and moltemplate.

License

Moltemplate is open source and publicly available at `http://moltemplate.org`. With the exception of one file (*ttree_lex.py*) moltemplate is available under the terms of the *MIT license*. The remaining file, (*ttree_lex.py*) is a modified version of (*shlex.py*) which is available under the *PSF license* (`https://docs.python.org/3/license.html`).

2 Installation

There are three ways to install moltemplate:

Installation Method 1 (pip)

If you are familiar with pip, you can install moltemplate by typing following command in the terminal/shell:

```
pip install moltemplate
```

If you receive an error regarding permissions, then run pip this way instead:

```
pip install moltemplate --user
```

Make sure that your default pip install bin directory is in your *PATH*. (This is usually something like ~/.local/bin/ or ~/anaconda3/bin/. If you have installed anaconda, your PATH should have been updated for you automatically.) Later, you can uninstall moltemplate using:

```
pip uninstall moltemplate
```

If you run into difficulty with pip, then try installing moltemplate into a temporary virtual environment by running these commands:

```
python -m venv ~/venv    #(or "virtualenv venv" if using python2)
source ~/venv/bin/activate
pip install moltemplate
#(now do something useful with moltemplate...)
```

(You will have to enter "source ~/venv/bin/activate" into a terminal beforehand every time you want to run moltemplate.) If all this fails, then try installing moltemplate by manually updating your $PATH environment variable. Instructions for doing that are included below.

Note: There are a large variety of detailed moltemplate examples which will be omitted if you install moltemplate this way. **Downloading the examples is strongly recommended.** You can do this either by using *git*, or by downloading them from the web page. (See below.) (The examples are located in the *examples/* subdirectory included with the download.)

Installation Method 2 (git/webpage + pip)

Obtaining Moltemplate

The most up-to-date version of moltemplate can be downloaded using **git**.

```
git clone https://github.com/jewettaij/moltemplate ~/moltemplate
```

Later, you can update the download to the latest version of moltemplate using:

```
git pull
```

(This is the recommended way to download moltemplate.)

Alternatively, if you don't have **git** installed, you can download moltemplate as a .tar.gz archive from `http://www.moltemplate.org` and then unpack it using:

```
tar -xzvf moltemplate_2020-2-22.tar.gz
```

(The date will vary from version to version.)

Then move the unpacked moltemplate directory to your home directory (~/) and run:

```
cd  ~/moltemplate
pip install .  # (or "pip install --user", if that fails)
```

As mentioned earlier, if you are having difficulty, try to installing moltemplate in a virtual environment instead. Using virtual environments is cleaner, and can avoid many of the common pitfalls that occur in computers with complex python installations. To do that, follow the instructions above (in Method 1) to start a virtual environment, and *then* run "pip install .".

Installation Method 3 (updating your PATH)

Alternatively, you can download the moltemplate files (as explained above) and edit your *PATH* variable. The *PATH* variable helps the shell (eg. *BASH*) find the programs you type into the terminal. You must edit the PATH variable to include the subdirectory where the moltemplate.sh script is located (eg. "~/moltemplate/moltemplate/scripts/"), as well as the directory containing the most of the python scripts (eg. "~/moltemplate/moltemplate/").

If you use the **BASH** shell, typically you would edit your ~/.bashrc file (or your ~/.bash_profile, or ~/.profile file) and append the following lines to that file:

```
export PATH="$PATH:$HOME/moltemplate/moltemplate"
export PATH="$PATH:$HOME/moltemplate/moltemplate/scripts"
```

If instead you use the **TCSH** shell, typically you would edit your ~/.cshrc, ~/.tcshrc, or ~/.login files and append the following lines:

```
setenv PATH "$PATH:$HOME/moltemplate/moltemplate"
setenv PATH "$PATH:$HOME/moltemplate/moltemplate/scripts"
```

Note: You may need to log out and then log back in again for the changes to take effect.

*Warning: Do not install moltemplate this way if you you plan to invoke moltemplate from within the python environment, **or** if you are using "vipster", "cellpack2moltemplate" or other software that has a moltemplate python dependency. In order to be able to be able to run "import moltemplate", as these programs do, moltemplate must be installed using pip (or setuptools).*

WINDOWS installation suggestions

You can install both moltemplate and LAMMPS in windows, but you will first need to install the *BASH* shell environment on your computer. I recommend installing **virtualbox**(https://www.virtualbox.org) in windows together with a (debian-based) linux distribution with a lightweight desktop such as **xubuntu**(https://xubuntu.org). Alternatively, if you are using Windows 10 or later, you can try installing the **Windows Subsystem for Linux (WSL)** (*which is text only*, https://docs.microsoft.com/en-us/windows/wsl) or **Hyper-V** (https://www.nakivo.com/blog/run-linux-hyper-v/). Otherwise, if you are using an older version of windows, try installing **CYGWIN** (https://www.cygwin.com/) instead.

To use LAMMPS and moltemplate, you will also need to install (and learn how to use) a text editor. (Word, Wordpad, and Notepad will not work.) If you are *NOT using WSL*, then you can use popular graphical text editors such as *Atom, Sublime, Notepad++, VSCode*, and the graphical versions of *emacs* and *vim*. (*Note:* Don't use these editors if you are using the WSL environment. Under WSL, these editors may cause file system corruption. Avoid them for now. (https://www.reddit.com/r/bashonubuntuonwindows/comments/6bu1d1/since_we_shouldnt_edit_files_

`stored_in_wsl_with/`) If you *ARE using WSL* then you are restricted to using non-graphical text editors which you can safely install and run from within the WSL terminal. These include: *nano*, *ne*, *emacs* (text version), *vim* (text version), and *jove*.

3 Quick reference *(skip on first reading)*

Note: New users should skip to section 4

3.1 Moltemplate commands

command	meaning

MolType {
 	
   content ...
 	
}
	Define a new type of molecule (or namespace) named *MolType*. The text enclosed in curly brackets (*content*) typically contains multiple write(), write_once() commands to define Atoms, Bonds, Angles, Coeffs, etc... *(If that molecule type exists already, then this will append additional* **content** *to its definition.)* (See the *SPCE*, *Monomer*, and *Butane* molecules, and the *TraPPE* namespace defined in sections 4.1, 6.1, 10.7, & 10.4.1.

mol_name = **new** *MolType*	Create (instantiate) a copy of a molecule of type *MolType* and name it *mol_name*. (See section 4.1.)
mol_name = **new** *MolType.xform()*	Create a copy of a molecule and apply coordinate transformation *xform()* to its coordinates. (See sections 4.2 and 3.3.)
molecules = **new** *MolType* [N].*xform()*	Create N copies of a molecule of type *MolType* and name them *molecules[0]*, *molecules[1]*, *molecules[2]*... Coordinates in each successive copy are cumulatively transformed according to *xform()*. (See sections 4.2, 8.1 and 3.3.) Multidimensional arrays are also allowed. (See section 8.6.)
molecules = **new** *MolType.xform1()* [***N***].*xform2()*	Apply coordinate transformations (*xform1()* to *MolType*, before making N copies of it while cumulatively applying *xform2()*. (See section 8.1 and 8.3.)

molecules = **new**
   random([*M1.xf1()*,
        M2.xf2(),
        M3.xf2(),...],
        [p_1, p_2, p_3,...],
        seed)
   [***N***].*xform()*
	Generate an array of N molecules randomly selected from *M1,M2,M3,...* with probabilities $p_1, p_2, p_3...$, using (optional) initial coordinate transformations *xf1()*, *xf2()*, *xf3*, ..., and applying transformation *xform()* cumulatively thereafter. This also works with multidimensional arrays. **You can directly specify the number of each type of molecule** by replacing the list of probabilities $[p_1, p_2, p_3 \ldots]$, with a list of integers $[n_1, n_2, n_3 \ldots]$. (See sections 8.4 and 8.8.)

NewMol = *OldMol*	Create a new molecule **type** based on an existing molecule type. Additional atoms (or bonds, etc...) can be added later to the new molecule using NewMol {*more content...*}. (See section 9.4.)
NewMol = *OldMol.xform()*	Create a new molecule **type** based on an existing molecule type, and apply coordinate transformation *xform()* to it. (See section 9.4.)

NewMol **inherits** *Mol1 Mol2* ... {
 	
   additional content ...
 	
}
	Define a new object **type** based one or more existing object types. Atom types, bond types, angle types (etc) which are defined in *Mol1*, or *Mol2*, ... are available inside the new object. *Additional content* (including more *write()* or *write_once()* or *new* commands) follows within the curly brackets. (See sections 9.4, 10.7, and 10.7.1)

MolType.xform()	Apply the coordinate transform *xform()* to the coordinates of the atoms in all molecules of type *MolType*. (See section 9.4.)
molecule.xform()	Apply the coordinate transform *xform()* to the coordinates in *molecule*. (Here *molecule* refers to a specific instance or copy of a particular molecule type. See sections 9 and 4.2.)
molecules[range].xform()	Apply the coordinate transform *xform()* to the coordinates of molecules specified by *molecule[range]*. (This also works for multidimensional arrays. See sections 8.5 and 9.)
delete *molecule*	Delete the *molecule* instance. (**delete** can also be used to delete atoms, bonds, angles, dihedrals, and improper interactions.) See section 9.3.
delete *molecules[range]*	Delete a range of molecules specified by *molecules[range]*. (This also works for multidimensional arrays. See sections 9.3 and 8.10.)

write_once('*file*') {
   text ...
}
	Write the text enclosed in curly brackets {...} to file *file*. The *text* can contain @variables which are replaced by integers. (See sections 5.1 and 5.2.)

write('*file*') {
   text ...
}
	Write the text enclosed in curly brackets {...} to file *file*. *This is done every time a new copy of this molecule is created using the "new" command.* The *text* can contain either @variables or $variables which will be replaced by integers. (See sections 5.1 and 5.2.)

Note: *file* names beginning with "Data " or "In " (such as "Data Atoms" or "In Settings") are inserted into the relevant section of the LAMMPS data file or input script. (See section 5.4.)
include *file*	Insert the contents of file *file* here. (Quotes optional.)
import *file*	Insert the contents of file *file* here, preventing circular (self-referential) inclusions. *(recommended)*
category *$catname($i_0$, Δ)* *or* **category** *@catname(i_0, Δ)*	Create a new category of counter variables starting at i_0 and incrementing by Δ. See section D.2 for details.
create_var { *$variable* } *or* **create_static_var** { *@variable* }	Create a variable specific to this molecule object. (**create_var** is typically used to create molecule-ID numbers that are shared between subunits of a larger molecule. See section 6.1. **create_static_var** is typically used to define shared @atom types.)

replace { *oldvariable newvariable* }	Allow alternate names for the same variable. This replaces all instances of *oldvariable* with *newvariable*. Both variable names must have a "@" prefix. This is typically used to reduce the length of long variables, for example to allow the shorthand "@atom:C2" to refer to "@atom:C2_bC2_aC_dC_iC" (See section 7.4.)
#*commented text*	All text following a "#" character is treated as a comment and ignored.

3.2   Common $ and @ variables

(See section 5.2 for details.)

variable type	meaning
$atom:*name*	A unique ID number assigned to atom *name* in this molecule. (Note: The *:name* suffix can be omitted if the molecule in which this variable appears only contains a single atom.)
@atom:*type*	A number which indicates an atom's *type* (typically used to lookup pair interactions.)
$bond:*name*	A unique ID number assigned to bond *name* (Note: The *:name* suffix can be omitted if the molecule in which this variable appears only contains a single bond.)
@bond:*type*	A number which indicates a bond's *type*
$angle:*name*	A unique ID number assigned to angle *name* (Note: The *:name* suffix can be omitted if the molecule in which this variable appears only contains a single angle interaction.)
@angle:*type*	A number which indicates an angle's *type*
$dihedral:*name*	A unique ID number assigned to dihedral *name* (Note: The *:name* suffix can be omitted if the molecule in which this variable appears only contains a single dihedral-angle interaction.)
@dihedral:*type*	A number which indicates a dihedral's *type*
$improper:*name*	A unique ID number assigned to improper *name* (Note: The *:name* suffix can be omitted if the molecule in which this variable appears only contains a single improper interaction.)
@improper:*type*	A number which indicates an improper's *type*
$*mol*:*name*	A unique molecule ID number. Typically all the atoms in molecule have the same molecule ID. (The ":*name*" suffix is optional. If omitted, the default *name* is ".".)
$*mol*:...	The ID number assigned to the molecule to which this object belongs (if applicable). See sections 6.1, 10.6.2, and appendix G.1.
*The numbers assigned to each variable are saved in the **output_ttree/ttree_assignments.txt** file*	
Advanced variable usage	
$*category*:**query**()	Query the current value of the counter in this *$category* without incrementing it. (The "*$category*" is usually either *$atom, $bond, $angle, $dihedral, $improper*, or *$mol*.) This is useful for counting the number of atoms, bonds, angles, molecules, etc... created so far.
@*category*:**query**()	Query the current value of the counter in this *@category* without incrementing it. (The "*@category*" is usually either *@atom, @bond, @angle, @dihedral*, or *@improper*.) This is useful for counting the number of atom types, bond types, angle types, etc... declared so far.)
@{*category:variable*} or ${*category:variable*}	Curly-brackets, **{}**, are used to refer to variables with non-standard delimiters or whitespace characters. (See section 5.6.)

13

@{category:*type*.rjust(n)} or @{category:*type*.ljust(n)} or ${category:*name*.rjust(n)} or ${category:*name*.ljust(n)}	Print the counter variable in a right-justified or a left-justified text-field of fixed width n characters. (This is useful for generating text files which require fixed-width columns.)

3.3 Coordinate transformations

(See sections 4.2) and 8.1) for details.)

suffix	meaning
.move(x,y,z)	Add numbers *(x,y,z)* to the coordinates of every atom
.rot(θ, x, y, z)	Rotate atom coordinates by angle θ around axis *(x,y,z)* passing through the origin. (Dipole directions are also rotated.)
.rot(θ, x, y, z, x_0, y_0, z_0)	Rotate atom coordinates by angle θ around axis pointing in the direction *(x,y,z)*, passing through the point (x_0, y_0, z_0). (This point will be a *fixed point.*)
$.rotvv(v_{1x}, v_{1y}, v_{1z}, v_{2x}, v_{2y}, v_{2z})$	Rotate atom coordinates with an angle which rotates the vector $\mathbf{v}_1$ to $\mathbf{v}_2$ (around an axis perpendicular to both $\mathbf{v}_1$ and $\mathbf{v}_2$). If you supply 3 additional numbers x_0, y_0, z_0, the axis of rotation will pass through this location.
.scale(ratio)	Multiply all atomic coordinates by *ratio*. (**Important:** *The scale() command does not update force-field parameters such as atomic radii or bond-lengths. Dipole magnitudes are affected.*)
$.scale(x_r, y_r, z_r)$	Multiply *x, y, z* coordinates by x_r, y_r, z_r, respectively
$.scale(ratio, x_0, y_0, z_0)$ or $.scale(x_r, y_r, z_r, x_0, y_0, z_0)$	You can supply 3 optional additional arguments x_0, y_0, z_0 which specify the point around which you want the scaling to occur. (This point will be a *fixed point.* If omitted, the origin is used.)
$.quat(a, b, c, d)$ $.quat(a, b, c, d, x_0, y_0, z_0)$	Rotate atom coordinates by the rotation corresponding to quaternion $a + b\mathbf{i} + c\mathbf{j} + b\mathbf{k}$ (around (x_0, y_0, z_0), if specified).
$.matrix(M_{1,1}, M_{1,2}, M_{1,3}, M_{2,1}, M_{2,2}, M_{2,3}, M_{3,1}, M_{3,2}, M_{3,3})$	Apply a general linear coordinate transformation. $$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} M_{1,1} & M_{1,2} & M_{1,3} \\ M_{2,1} & M_{2,2} & M_{2,3} \\ M_{3,1} & M_{3,2} & M_{3,3} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Note: **Multiple transformations can be chained together into a compound operation.**
(For example: ".*scale*(2.0).*rot*(45.2, 1, 0, 0).*move*(25.0, 0, 0)")
These are evaluated from left-to-right. (See section 8.1.)

$push(\text{rot}(152.3, 0.79, 0.43, -0.52))$ monomer1 = new Monomer $push(\text{move}(0.01, 35.3, -10.1))$ monomer2 = new Monomer $pop()$ $pop()$	Coordinate transformations introduced using the *push()* command are applied to molecules instantiated later (using the *new*) command, and remain in effect until they are removed using the *pop()* command. (And transformations appearing in arrays accumulate as well, but do not need to be removed with *pop()*.) In this example, the first transformation, "rot()", is applied to both "monomer1" and "monomer2". The last transformation, "move()", is applied after "rot()" and only acts on "monomer2".

3.4   moltemplate.sh command line arguments:

argument	meaning
-atomstyle *style*	Inform moltemplate which atom_style you are using. (*style* is "full" by default). Other styles like "molecular" or "hybrid full dipole" are supported. For custom atom styles, you can also specify the list of column names manually. For example: **-atomstyle "molid x y z atomid atomtype mux muy muz"** Atom styles should be enclosed in quotes (").
-raw coords.raw	Read all of the atomic coordinates from an external RAW file. (RAW files are simple 3-column ASCII files contain X Y Z coordinates for every atom, separated by spaces.)
-xyz coords.xyz	Read all of the atomic coordinates from an external XYZ file (XYZ files are 4-column ascii files in ATOMTYPE X Y Z format. The first column, ATOMTYPE, is skipped. The first line should contain the number of atoms. The second line is skipped. See section 4.2.)
-pdb coords.pdb	Read all of the atomic coordinates from an external PDB file (Periodic boundary conditions are also read, if present. The order of atoms in the PDB file must match the order that the atoms appear in the data file, which matches the order they appear in the LT file. See section 4.2.)
-dump coords.lammpstrj	Read all of the atomic coordinates from a LAMMPS dump (trajectory) file. (If ellipsoids are present, the dump file must be formatted in the following order: "id type xu yu zu c_q[1] c_q[2] c_q[3] c_q[4] ... " where "q" is defined by "compute q all property/atom quatw quati quatj quatk".)
-a '*variable value*'	Assign *variable* to *value*. (The *variable* should begin with either a @ character or a $ character. Single-quotes and a space separator are required. See appendix D.1.)
-a bindings_file'	The variables in column 1 of *bindings_file* (which is a text file) will be assigned to the values in column 2 of that file. (This is useful when there are many variable assignments to make. See appendix D.1.)
-b '*variable value*' *or* -b *bindings_file*	Assign variables to values. Unlike assignments made with "-a", assignments made using "-b" are non-exclusive. (They may overlap with other variables in the same category. See appendix D.1.)
-overlay-bonds -overlay-angles -overlay-dihedrals -overlay-impropers	By default moltemplate overwrites duplicate bonded interactions which involve the same set of atoms. These flags disable that behavior. This can be useful when you want to superimpose multiple angular or dihedral forces on the same set of atoms (eg. to enable more complex force fields). Note: Each duplicate must still be given an unique $bond, $angle, $dihedral, $improper style variable name.

-nocheck	Do *not* check for common LAMMPS/moltemplate syntax errors. (This might be useful when using moltemplate with simulation software other than LAMMPS, *or* to build systems which need new non-standard LAMMPS features.)
-checkff	This forces moltemplate.sh to check that there are valid angle and dihedral interactions defined for every 3 or 4 consecutively bonded atoms in the system (defined in "Data Angles By Type" and "Data Dihedrals By Type" sections).
-vmd	Invoke VMD after running moltemplate to view the system you have just created. (VMD must be installed. See sections 4.3, C for details.)
-dihedral-sym file.py -improper-sym file.py -bond-symmetry file.py -angle-symmetry file.py	Normally moltemplate.sh reorders the atoms in each bond, angle, dihedral, and improper interaction before writing them to the DATA file in order to help avoid duplicate interactions between the same atoms if listed in different but equivalent orders. Sometimes this is undesirable. ***To disable this behavior, set "file.py" to "None".*** You can also manually choose alternate symmetry rules for unusual force fields. (Such as class2 force fields, dihedral_style spherical, etc... For an example of the file format for "file.py", see the "nbody_Impropers.py" file.)
-molc	Helpful additional post-processing for users of the **MOLC** coarse-grained model
-short-comment-names -full-comment-names	Moltemplate writes atom type names in the comments following the "Masses" section of a LAMMPS data file. These two arguments control whether or not the *short* or *full* versions of the atom type names are printed there. (Default: short. See section 5.2.3 for details.)
-forbid-wildcards	Forbid the use of "*" and "?" characters in "pair_coeff", "bond_coeff", "angle_coeff", "dihedral_coeff", and "improper_coeff" commands. (eg: "bond_coeff @bond:CH?? ...", "pair_coeff @atom:C* @atom:C* ...". These are allowed by default.)

4 Introductory tutorial

Summary

Moltemplate is based on a very simple text generator (wrapper) which repetitively copies short text fragments into one (or more) files and keeps track of various kinds of counters.

LAMMPS is a powerful but complex program with many contributors. Moltemplate is a front-end for LAMMPS. Moltemplate users will have to tackle the same steep learning-curve (and occasional bugs) that other LAMMPS users must face. Moltemplate files (LT files) share the same file format and syntax structure as LAMMPS DATA files and INPUT scripts. Moltemplate will attempt to correct user mistakes, however users must still learn LAMMPS syntax and write LT files which obey it. For users who are new to LAMMPS, the easiest way to do this is to modify an existing example (such as the water box example in this section). (The official LAMMPS documentation `http://lammps.sandia.gov/doc/Manual.html` is an excellent reference to look up LAMMPS commands you see in these examples that you are not familiar with.)

4.1 Simulating a box of water using moltemplate and LAMMPS

Figure 1: Coordinates of a single water molecule in our example. (Atomic radii not to scale.)

Here we show an example of a lammps-template file for water. (The settings shown here are borrowed from the simple-point-charge [7] SPC/E model.) In addition to coordinates, topology and force-field settings, "LT" files can optionally include any other kind of LAMMPS settings including RATTLE constraints, k-space settings, and even group definitions.

```
# (NOTE: Text following '#' characters are comments)
#
# file "spce_simple.lt"
#
#    h1     h2
#      \   /
#        o
#

SPCE {

  ## Atom properties and bond topology go in various "Data ..." sections

  # We selected "atom_style full". That means we use this column format:
```

18

```
# atomID     molID    atomType  charge  coordX     coordY     coordZ

write("Data Atoms") {
  $atom:o   $mol:w  @atom:O  -0.8476  0.0000000 0.000000  0.00000
  $atom:h1  $mol:w  @atom:H   0.4238  0.8164904 0.5773590 0.00000
  $atom:h2  $mol:w  @atom:H   0.4238  -0.8164904 0.5773590 0.00000
}

# Variables beginning with $ or @ will be replaced by numbers LAMMPS will
# eventually read.  Each of the three atoms" will be assigned unique
# atomIDs (denoted here by "$atom:o", "$atom:h1", "$atom:h2"), even if
# they belong to different molecules.  However, the atom types
# (denoted "@atom:O", "@atom:H") are shared for atoms in all molecules.
# All 3 atoms share same molID number (represeted here by "$mol:w")
# however that number is different for different water molecules.

write_once("Data Masses") {
  # atomType  mass
  @atom:O    15.9994
  @atom:H    1.008
}

write("Data Bonds") {
  #  bondID  bondType  atomID1  atomID2
  $bond:oh1  @bond:OH  $atom:o  $atom:h1
  $bond:oh2  @bond:OH  $atom:o  $atom:h2
}

write("Data Angles") {
  # angleID  angleType  atomID1  atomID2 atomID3
  $angle:hoh @angle:HOH $atom:h1 $atom:o $atom:h2
}

# --- Force-field parameters go in the "In Settings" section: ---

write_once("In Settings") {
  # -- Non-bonded (Pair) interactions --
  #          atomType1 atomType2  parameter-list (epsilon, sigma)
  pair_coeff  @atom:O  @atom:O    0.1553 3.166
  pair_coeff  @atom:H  @atom:H    0.0    2.058
  # (mixing rules determine interactions between types @atom:O and @atom:H)

  # -- Bonded interactions --
  #            bondType   parameter list (k_bond, r0)
  bond_coeff   @bond:OH    1000.00 1.0
  #            angleType  parameter-list (k_theta, theta0)
  angle_coeff  @angle:HOH 1000.0   109.47
```

```
    # Group definitions and constraints can also go in the "In Settings" section
    group spce type  @atom:O  @atom:H
    fix fRATTLE spce rattle 0.0001 10 100 b @bond:OH a @angle:HOH
    # (lammps quirk: Remember to "unfix fRATTLE" during minimization.)
  }


  # LAMMPS supports a large number of force-field styles. We must select
  # which ones we need. This information belongs in the "In Init" section.

  write_once("In Init") {
    units        real                    # angstroms, kCal/mole, Daltons, Kelvin
    atom_style   full                    # select column format for Atoms section
    pair_style   lj/charmm/coul/long 9.0 10.0 10  # params needed: epsilon sigma
    bond_style   harmonic                # parameters needed: k_bond, r0
    angle_style  harmonic                # parameters needed: k_theta, theta0
    kspace_style pppm 0.0001             # long-range electrostatics sum method
    pair_modify  mix arithmetic          # using Lorenz-Berthelot mixing rules
  }


} # SPCE
```

Words which are preceded by "$" or "@" characters are counter variables and will be replaced by integers. (See section 5.2 for details.) Users can include SPCE water in their simulations using commands like these:

```
# -- file "system.lt" --
import "spce_simple.lt"
wat = new SPCE [1000]
```

You can now use "moltemplate.sh" to create simulation input files for LAMMPS

```
moltemplate.sh -pdb coords.pdb -atomstyle "full" system.lt
```

This command will create lammps input files for the molecular system described in "system.lt", using the desired atom style ("full" by default). In this example, moltemplate is relying on an external file ("coords.pdb") to supply the atomic coordinates of the water molecules, as well as the periodic boundary conditions. *Note:* The order of atoms in the PDB file must match the order that the atoms appear in the LT file. (So in this example, the oxygen atom in each water molecule in the PDB file must precede the two hydrogen atoms in that molecule.) Coordinates in XYZ format are also supported using "-xyz coords.xyz".

Details

Note that since XYZ files lack boundary information, you must also include a "Boundary" section in your ".lt" file, as demonstrated in section 4.2. In both cases, the order of the atom types in a PDB or XYZ file (after sorting) should match the order they are created by moltemplate (which is determined by the order of the "new" commands in the LT file). Unfortunately this may require careful manual editing of the PDB or XYZ file.

4.2   Coordinate generation

It is not necessary to provide a separate file with atomic coordinates. It is more common to manually specify the location (and orientation) of the molecules in your system using the ".move()" and ".rot()" commands in the LT file itself (discussed in section 6). For example you can replace the line:

```
wat = new SPCE [1000]
```

from the example above with 1000 lines:

```
wat1    = new SPCE
wat2    = new SPCE.move(3.1034, 0.00, 0.00)
wat3    = new SPCE.move(6.2068, 0.00, 0.00)
wat4    = new SPCE.move(9.3102, 0.00, 0.00)
   :             :
wat1000 = new SPCE.move(31.034, 31.034, 31.034)
```

Specifying geometry this way is tedious. Alternatively, moltemplate has simple commands for arranging multiple copies of a molecule in periodic, crystalline, toroidal, and helical 1-D, 2-D, and 3-D lattices. For example, you can generate a simple cubic lattice of $10 \times 10 \times 10$ water molecules (with a 3.1034 Angstrom spacing) using a single command (which in this example we split into multiple lines)

```
wat  = new SPCE [10].move(0.0, 0.0, 3.1034)
                [10].move(0.0, 3.1034, 0.0)
                [10].move(3.1034, 0.0, 0.0)
```

(See section 6 for more details and examples.) This will create 1000 molecules with names like "wat[0][0][0]", "wat[0][0][1]",..., "wat[9][9][9]". You can always access individual atomIDs, molIDs, bondIDs, angleIDs, and dihedralIDs (if present), for any molecule elsewhere in your LT files using this notation: "$atom:wat[2][3][4]/h1", "$bond:wat[0][5][1]/oh1", "$angle:wat[2][8][3]/hoh", "$mol:wat[0][1][2]/w". This allows you to define interactions which link different molecules together (see section 6).

A list of available coordinate transformations is provided in section 3.3.

Boundary Conditions:

LAMMPS simulations have finite volume and are usually periodic. We must specify the dimensions of the simulation boundary using the "write_once("Data Boundary")" command.

```
write_once("Data Boundary") {
   0.0  31.034  xlo xhi
   0.0  31.034  ylo yhi
   0.0  31.034  zlo zhi
}
```

This is usually specified in the outermost LT file ("system.lt" in this example). *(Note: Boundary conditions do not have to be rectangular or even*

periodic. For triclinic cells, additional "xy", "xz", and "yz" tilt parameters can be added. For details, lookup the "read_data" and "boundary" commands in the official LAMMPS documentation.)

This system is shown in figure 2a). After you have specified the geometry, then you can run moltemplate.sh this way:

```
moltemplate.sh -atomstyle "full" system.lt
```
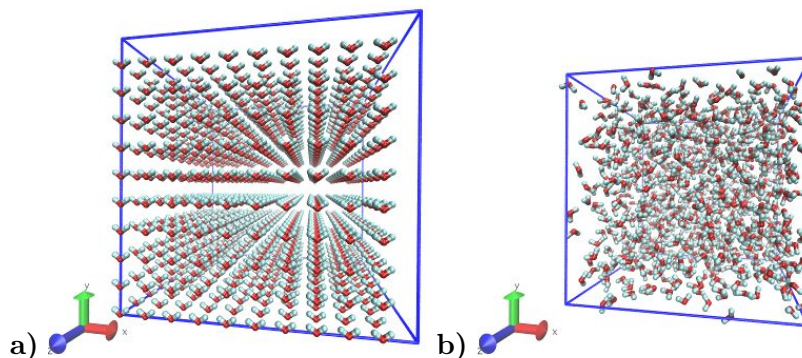

Figure 2: A box of 1000 water molecules (before and after pressure equilibration), generated by moltemplate and visualized by VMD with the topotools plugin. (The VMD console commands used for visualization were: "topo readlammpsdata system.data full", "animate write psf system.psf", "pbc wrap -compound res -all", and "pbc box". See sections 4.3, and appendix C for details.

4.3   Visualization using VMD & topotools

When you run moltemplate, it generates a LAMMPS *data* file. This file is usually called "system.data". Geometric information, and bonded topology are stored in this file. After you have run moltemplate, you should look at your system to check it for mistakes. Problems can easily occur with overlapping atoms (missing molecules), periodic boundaries, incorrectly bonded atoms, incorrect rotation and movement. Sometimes many iterations of running moltemplate and visualization are necessary.

Optional: If you have VMD installed, you can automatically visualize the system you have just created automatically by invoking moltemplate with the ***-vmd*** command line argument. (In other words invoke moltemplate.sh using *moltemplate.sh -vmd* instead of *moltemplate.sh*. VMD must be installed.) If you don't use the -vmd command line argument, you can always view the system in VMD later manually. For instructions how to do that, keep reading...

Some very basic instructions how to use VMD are provided below: *(Note: These instructions were written for VMD 1.9 and topotools 1.2)*

To view a *data* file:

 a) start VMD

 b) from the menu, select **Extensions→Tk Console**

c) enter:

```
topo readlammpsdata system.data full
animate write psf system.psf
```

The first command will display all of the atoms and bonds in your system in VMD's 3-D window. (We use "**full**" because we are using the "full" atom_style in this particular example. If you are using a different atom_style, then change the command above accordingly.)

The second command will create a PSF file ("system.psf") which will be useful later for viewing a trajectory file created during a LAMMPS simulation. (See section 4.5.)

Most likely, atoms and bonds will be represented by ugly dots and lines by default. To change the way molecules are displayed, control their color, display periodic boundaries, and wrap atomic coordinates, read the short VMD tutorial in appendix C.

(Note: As of 2019-9-03, VMD does not have built-in support for exotic atom_styles such as ellipsoids and dipoles, but their are 3rd-party scripts, plugins and settings you can use. Search the VMD and LAMMPS mailing lists for help.)

4.4 Running a LAMMPS simulation (after using moltemplate)

To run a simulation of one or more molecules, LAMMPS requires an *input script* and a *data file*. Input scripts typically contain force field styles, parameters and run settings. (They sometimes also contain atom coordinates.) Data files typically contain atom coordinates and bonded topology data. (They sometimes also contain force-field parameters.)

Moltemplate will create the following files: "system.data", "system.in", "system.in.init", "system.in.settings", (and possibly other files including "system.in.coords"). These are LAMMPS input/data files, and they can be run in LAMMPS with minimal modification (see below). The main input script file is named "system.in", and it usually contains just three lines:

```
include   "system.in.init"
read_data "system.data"
include   "system.in.settings"
```

To *run* a simulation, you will have to edit this file in order to add a couple of run commands. These commands tell LAMMPS about the simulation conditions you want to use (temperature, pressure), how long to run the simulation, how to integrate the equations of motion, and how to write the results to a file (file format, frequency, etc). Moltemplate.sh can not do this for you. Some simple examples (which you can paste into your input script) are provided in the *online examples* which can be downloaded from `http://moltemplate.org`. (These example input scripts typically have names like "run.in.nvt" and "run.in.npt".)

In addition to the examples, an introduction to LAMMP input scripts is provided at these links: `http://lammps.sandia.gov/doc/Section_commands.html#cmd_1`. `http://lammps.sandia.gov/doc/Section_howto.html` and `http://lammps.sandia.gov/doc/Section_howto.html#howto_15`

Here is a list of basic input script commands used in the moltemplate examples (and links to their documentation):

run `http://lammps.sandia.gov/doc/run.html`

timestep `http://lammps.sandia.gov/doc/timestep.html`

thermo `http://lammps.sandia.gov/doc/thermo.html`

dump `http://lammps.sandia.gov/doc/dump.html`

read_data `http://lammps.sandia.gov/doc/read_data.html`

restart `http://lammps.sandia.gov/doc/restart.html`

include `http://lammps.sandia.gov/doc/include.html`

fix nve `http://lammps.sandia.gov/doc/fix_nve.html`

fix nvt `http://lammps.sandia.gov/doc/fix_nh.html`

fix npt `http://lammps.sandia.gov/doc/fix_nh.html`

fix langevin `http://lammps.sandia.gov/doc/fix_langevin.html`

fix `http://lammps.sandia.gov/doc/fix.html`

group `http://lammps.sandia.gov/doc/group.html`

compute `http://lammps.sandia.gov/doc/compute.html`

print `http://lammps.sandia.gov/doc/print.html`

variable `http://lammps.sandia.gov/doc/variable.html`

rerun `http://lammps.sandia.gov/doc/rerun.html`

fix rattle `http://lammps.sandia.gov/doc/fix_shake.html`

fix shake `http://lammps.sandia.gov/doc/fix_shake.html`

fix rigid `http://lammps.sandia.gov/doc/fix_rigid.html`

In addition, all users should be familiar with the following commands: (These appear in the "In Init" section of most LT files.)

atom_style `http://lammps.sandia.gov/doc/atom_style.html`

pair_style `http://lammps.sandia.gov/doc/pair_style.html`

bond_style `http://lammps.sandia.gov/doc/bond_style.html`

angle_style `http://lammps.sandia.gov/doc/angle_style.html`

4.5 Visualizing Trajectories

After you have run a simulation in LAMMPS, there are several programs which can visualize the system. If you have saved your trajectory in LAMMPS "dump" format, later you can view it in VMD [4]. For the purpose of viewing trajectories in LAMMPS, I recommend using the following style of "dump" commands in the LAMMPS input-script that you use when you run LAMMPS:

```
dump 1 all custom 1000 DUMP_FILE.lammpstrj id mol type x y z ix iy iz
```

(The "all" and "1000", refer to the atom selection and save interval, which may differ depending on the kind of simulation you are running. See `http://lammps.sandia.gov/doc/dump.html` for details.)

Once you have a dump file, you can view it in VMD using:

a) Start VMD From the menu in the upper-left, select **File→New Molecule**

b) Browse to select the PSF file you created above, and load it. (Don't close the window yet.)

c) Browse to select the trajectory file. If necessary, for "file type" select: "LAMMPS Trajectory". Click on **OK**.

d) Click on the **Load** button.

Again, to customize molecule appearance, display periodic boundary conditions and wrap molecule coordinates, see the commands discussed in appendix C.

*(Note: VMD may not be able to correctly visualize simulations which do not preserve the number of atoms and bonds over time, such as those run using **fix bond/create**, **fix bond/break**, or **fix gcmc**.)*

5 Overview

5.1 Basics: The *write()* and *write_once()* commands

Each LT file typically contains one or more "write" or "write_once" commands. These commands have the following syntax

```
write_once(filename) {text_block}
```

This creates a new file with the desired file name and fills it with the text enclosed in curly brackets {}. Text blocks usually span multiple lines and contain counter variables (beginning with "@" or "$"). which are replaced with numbers. However the "write()" command will repeatedly append the same block of text to the file every time the molecule (in which the write command appears) is generated or copied (using the "new" command, after incrementing the appropriate counters, as explained in 5.2.2).

5.2 Basics: counter variables

Words following a "@" or a "$" character are *counter variables*. (These are not to be confused with *LAMMPS variables* `http://lammps.sandia.gov/doc/variable.html`). By default, *all counter variables are substituted with a numeric counter* before they are written to a file. These counters begin at 1 (by default), and are incremented as the system size and complexity grows (see below).

These words typically contain a colon (:) followed by more text. The text preceding this colon is the *category name*. (For example: "$atom:", "$bond:", "$angle:", "@atom:", "@bond:", "@angle:") Variables belonging to different categories are counted independently.

Users can override these assignment rules and create custom categories. (See appendices D.1 and D.2 for details.)

5.2.1 Static counters begin with "@"

"@" variables generally correspond to *types*: such as atom types, bond types, angle types, dihedral types, improper types. These are simple variables and they assigned to unique integers in the order they are read from your LT files. Each uniquely named variable in each category is assigned to a different integer. For example, "@bond:" type variables are numbered from "1" to the number of *bond types*. (Pairs of bonded atoms are assigned a *bond type*. Later, LAMMPS will use this integer to lookup the bond-length and Hooke's-law elastic constant describing the force between these two atoms.)

5.2.2 Instance counters begin with "$"

On the other hand, "$" variables correspond to unique ID numbers: atom-IDs, bond-IDs, angle-IDs, dihedral-IDs, improper-IDs, and molecule-IDs. These variables are created whenever a copy of a molecule is created (using the "new" command). If you create 1000 copies of a water molecule using a command like

```
wat = new SPCE[10][10][10]
```

then moltemplate creates 3000 "$atom" variables with names like

```
$atom:wat[0][0][0]/o
$atom:wat[0][0][0]/h1
$atom:wat[0][0][0]/h2
$atom:wat[0][0][1]/o
$atom:wat[0][0][1]/h1
$atom:wat[0][0][1]/h2

  ⋮

$atom:wat[9][9][9]/o
$atom:wat[9][9][9]/h1
$atom:wat[9][9][9]/h2
```

5.2.3   Variable names: short-names *vs.* full-names

In the example above, the $ variables have full-names like "$atom:wat[8][3][7]/h1",
not "$atom:h1". However inside the definition of the water molecule, you
don't specify the full name. You can refer to this atom as "$atom:h1". Like-
wise, the full-name for the @atom variables is actually "@atom:SPCE/H",
not "@atom:H". However inside the definition of the water molecule, you
typically use the shorthand notation "@atom:H".

5.2.4   Numeric substitution

Before being written to a file, every variable (either $ or @) with a unique
full-name will be assigned to a unique integer, starting at 1 by default.

   The various $atom variables in the water example will be substituted
with integers from 1 to 3000 (assuming no other molecules are present).
But the "@atom:O" and "@atom:H" variables (which are shorthand for
"@atom:SPCE/O" and "@atom:SPCE/H") will be assigned to to "1" and
"2" (again, assuming no other molecule types are present).

   So, in summary, @ variables increase with the *complexity* of your system
(IE the number of molecule types or force-field parameters), but $ variables
increase with the *size* of your system.

5.2.5   Variable scope

This effectively means that all variables are specific to local molecules they
were defined in. In other words, an atom type named "@atom:H" in-
side the "SPCE" molecule, will be assigned to a different number than
an atom named "@atom:H" in an "Arginine" molecule. This is because
the two variables will have different *full* names ("@atom:SPCE/H", and
"@atom:Arginine/H").

Sharing atom types or other variables between molecules

There are several ways to share atom types between two molecules. The
recommended way is to define them in a separate file and refer to them
when needed. This approach is demonstrated in section 6.1.

   *(Alternately, you can define them outside the current molecule defini-
tion, and use file-system-path-like syntax ("../", or "../../" or "/") to access
atoms (or molecules) outside of the current molecule. For example, two dif-
ferent molecule types can share the same type of hydrogen atom by referring
to it using this syntax: "@atom:../H". For details, see section 10.6. and
appendix G.1.)*

5.3   Troubleshooting using the *output_ttree* directory

Users can see what numbers were assigned to each variable by inspecting the
contents of the "output_ttree" subdirectory created by moltemplate. Unfor-
tunately, it not unusual for LAMMPS to crash the first time you attempt to
run it on a DATA file created by moltemplate. This often occurs if you failed
to spell atom types and other variables consistently. The LAMMPS error

message (located at the end of the "log.lammps" file created by LAMMPS) will help you determine what type of mistake you made. (For example, what type of variable was misspelled or placed in the wrong place?)

To help you, the "output_ttree" directory contains a file named "ttree_assignments.txt". This is a simple 2-column text file containing a list of *all* of the variables you have created in one column, and the numbers they were assigned to in the second column. (There is also a comment on each line beginning with a "#" character which indicates the file and line number where this variable is first used.)

The "output_ttree" directory also contains all of the files that you created. The versions with a ".template" extension contain text interspersed with *full* variable names (before numeric substitution). (A spelling mistake, like using "$atom:h" when you meant to say "$atom:h1" or "@atom:H" will show up in these files if you inspect them carefully.) This can help you identify where the mistake occurred in your LT files.

Once a molecular system is debugged and working, users can ignore or discard the contents of this directory.

5.4 "Data" and "In"

Again, LAMMPS requires an *input script* and a *data file* to run. *Moltemplate's job is to generate these files. Input scripts* typically contain force-field styles, parameters and run settings *Data files* typically contain atom coordinates and bonded topology data.

If you are familiar with LAMMPS, you may have noticed the file names above (in the example from section 4.1) sound suspiciously like sections from LAMMPS data files or input scripts, such as "Data Boundary", "Data Atoms", "Data Bonds", "Data Masses", "Data Angles", "Data Dihedrals", "Data Impropers", "In Init", "In Settings"). All files whose names begin with "In " or "Data " are special. For the user's convenience, the moltemplate.sh script copies the contents of these files into the corresponding section ("Atoms", "Bonds", "Angles", etc.) of the DATA file or INPUT scripts generated by moltemplate ("system.data", "system.in.settings", etc). (Then the original files are moved to the "output_ttree/" directory, in an effort to clean things up and hide them from view.) Users can create their own custom sections to a LAMMPS data file. (See section 5.6.

More generally, the "write()" and "write_once()" commands can be used to create any other files you may need to run your simulations, which refer to the same *@atom* and *@bond* types. (See section 5.5 for an example.)

5.5 *(Advanced)* Using moltemplate to generate auxiliary files

The following excerpt from an LT file creates a file named "system.in.sw". (It contains parameters for the "sw" pair style. This exotic many-body pair style requires a large number of parameters, which are read from a separate file.) This "system.in.sw" file file will be read later when you run the simulation. (The pair_coeff command below tells LAMPS to read that file.)

```
write_once("system.in.sw") {
  mW mW mW 6.189 2.3925 1.8 23.15 1.2 -0.33333 7.04956 0.602224 4 0 0
}
write_once("In Settings") {
  pair_coeff * * sw system.in.sw mW NULL NULL NULL
}
```

As new force-field styles and/or fixes are added to LAMMPS, the files they depend on can be embedded in an LT file in this way.

5.6 *(Advanced)* Making custom DATA sections

Suppose that in the future, the format of the LAMMPS DATA file changes so that it now becomes necessary to supply a new section named "Foo Fee Fum", for example. You could do that using this command:

```
write_once("Data Foo Fee Fum") {
  File contents goes here. (These files can contain
  atom counters and/or other counter variables).
}
```

This way moltemplate copy this text into the "Foo Fee Fum" section at the end of the DATA file it is constructing. This allows users to adapt to future changes in the LAMMPS data file format.

Does "@atom:H" conflict with "$atom:H"?

No. It is okay for static(@) and instance($) variables to share the same names. (Moltemplate considers them distinct variables and they will be assigned independently.)

Addional Details

Variable and molecule names can include unicode characters. They can also include some whitespace characters and other special characters by using backslashes and curly-brackets, for example: "@{atom: CA }" and "@atom:\ CA\ ". Curly-brackets are useful to clarify when a variable name begins and ends, such as in this example: "@{atom:C}*@{atom:H}". This prevents the "*" character from being appended to the end of the "C" variable name. (Note that using the "*" character in any of the *coeff* commands within moltemplate is discouraged. See section 11.)

 (Unicode is supported.)

6   Object composition and coordinate generation

Objects can be connected together to form larger molecule objects. These objects can be used to form still larger objects. As an example, we define a small 2-atom molecule named "Monomer", and use it to construct a short polymer ("Polymer").
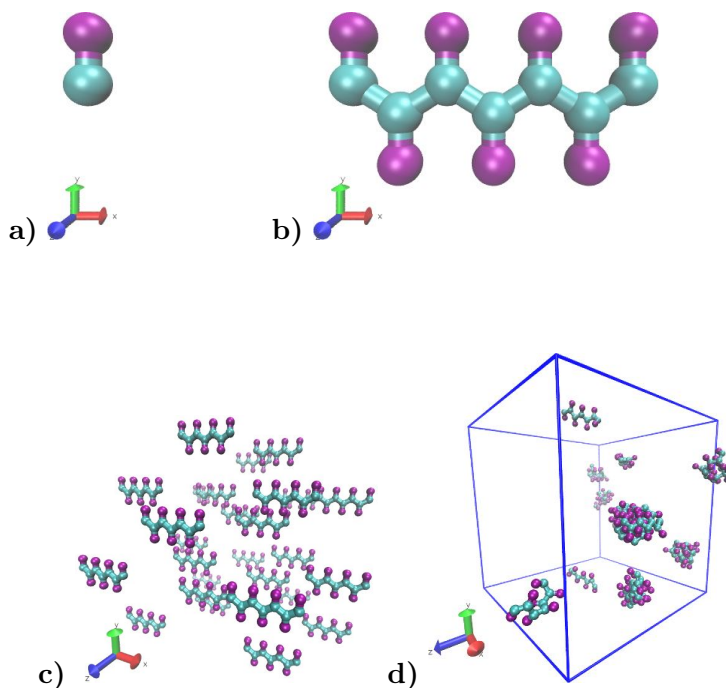
Figure 3: **a)-b)** *Building a complex system from small pieces:* Construction of a polymer (**b**) out of smaller (2-atom) subunits (**a**) using composition and rigid-body transformations. Bonds connecting different monomer together (blue) must be declared explicitly, but angle and dihedral interactions will be generated automatically. See section 6.1 for details. **c)** An irregular lattice of short polymers. (See section 8.6.) **d)** The same system after 100000 time steps using Langevin dynamics. (The VMD console commands used for visualization were: "topo readlammpsdata system.data full", "animate write psf system.psf", "pbc wrap -compound res -all", and "pbc box". See sections 4.3, and C for details.

6.1 Building a large molecule from smaller pieces

Consider the following simple 2-atom dumbell-shaped molelule ("Monomer")

```
# -- file "monomer.lt" --

import "forcefield.lt"   # contains force-field parameters

Monomer inherits ForceField {

  write("Data Atoms") {
    # atomId molId   atomType    charge    x       y         z
    $atom:ca $mol:... @atom:CA   0.0    0.000  1.0000    0.0000000
    $atom:r  $mol:... @atom:R    0.0    0.000  4.4000    0.0000000
  }
  write("Data Bonds") {
    # bond-id    bond-type        atom-id1   atom-id2
    $bond:cr     @bond:Sidechain  $atom:ca   $atom:r
  }
}
```

Soon will use it to construct a polymer ("Polymer") *Note: The ellipsis notation used here "$mol:...". warns moltemplate that the "Monomer" molecule may be part of a larger molecule. (This is explained in more detail in section 10.6.2.) (Note: The meaning of "inherits ForceField" will be explained below in section 7.1)*

In this example we will define two kinds of molecule objects: "Monomer", and "Polymer" (*defined later*).

Building a simple polymer

We construct a short polymer by making 7 copies of "Monomer", rotating and moving each copy:

```
# -- file "polymer.lt" --

import "monomer.lt"  #(defines "Monomer" and "ForceField")

Polymer inherits ForceField {

  # The next line is optional:
  create_var {$mol}  #(force all Monomers to share the same molecule-ID)

  # Now create some monomers

  mon1 = new Monomer      #(no need to move the first monomer)
  mon2 = new Monomer.rot(180.0, 1,0,0).move(3.2,0,0)
  mon3 = new Monomer.rot(360.0, 1,0,0).move(6.4,0,0)
  mon4 = new Monomer.rot(540.0, 1,0,0).move(9.6,0,0)
  mon5 = new Monomer.rot(720.0, 1,0,0).move(12.8,0,0)
```

```
  mon6 = new Monomer.rot(900.0, 1,0,0).move(16.0,0,0)
  mon7 = new Monomer.rot(1080.0, 1,0,0).move(19.2,0,0)

  # Now, link the monomers together this way:
  write("Data Bonds") {
    $bond:backbone1  @bond:Backbone  $atom:mon1/ca  $atom:mon2/ca
    $bond:backbone2  @bond:Backbone  $atom:mon2/ca  $atom:mon3/ca
    $bond:backbone3  @bond:Backbone  $atom:mon3/ca  $atom:mon4/ca
    $bond:backbone4  @bond:Backbone  $atom:mon4/ca  $atom:mon5/ca
    $bond:backbone5  @bond:Backbone  $atom:mon5/ca  $atom:mon6/ca
    $bond:backbone6  @bond:Backbone  $atom:mon6/ca  $atom:mon7/ca
  }
}
```

The position and orientation of each copy of "Monomer" is specified af-
ter the "new" statement. Each "new" statement is typically followed by
a chain of move/rotate/scale functions separated by dots, evaluated left-
to-right (optionally followed by square brackets and then more dots). For
example, "mon2" is a copy of "Monomer" which is first rotated 180 degrees
around the X axis (denoted by "1,0,0"), and **then** moved in the (3.2,0,0)
direction. (The last three arguments to the "rot()" command denote the
axis of rotation, which does not have to be normalized.) (A list of available
coordinate transformations is provided in section 3.3.)

   *(Note: Although we did not do this here, it is sometimes convenient
to represent polymers as 1-dimensional arrays. See sections 8 and 8.4 for
examples.)*

   To bond atoms in different molecules or molecular subunits together, we
used the write("Data Bonds") command to append additional bonds to the
system.

7 Force Fields

This is a short chapter describing the features of the moltemplate language
that enable users to create and store their own custom force-fields in LT
format.

   This is not a tutorial explaining how to use popular all-atom force-fields
(like OPLSAA or GAFF2) in your simulation. *(Perhaps later, I will add
more information on this worthy topic. For now, the best way to learn
to build realistic all-atom simulations is to download moltemplate and its
examples. Then modify an example which is similar to what you want to
simulate.)*

7.1 Bonded interactions *by type*

In the polymer example in the previous chapter, we did *not* provide a list of
all the angle, dihedral, and improper forces acting on the atoms in the poly-
mer. We *could* have listed them, however there are usually many of them. It
is often more convenient to provide moltemplate with instructions to help it

automatically determine which atoms participate in 3-body and 4-body angle interactions, and what force field parameters to assign to them. We will do that below using the following commands: "write_once("Data Angles By Type")", "write_once("Data Dihedrals By Type")", and "write_once("Data Impropers By Type")"

Furthermore, since many different kinds molecules often share the same rules for creating 3-body and 4-body angle interactions, it is convenient to organize all of this information together into one place (for example, an object named "ForceField"). A "ForceField" object will typically include a long list of "write_once("Data Angles/Dihedrals/Impropers By Type")" commands, as well as force field parameters and related atom type properties. It's also a good idea to store force-field objects in a separate file (eg "forcefield.lt", "oplsaa.lt", "gaff2.lt", "compass.lt", etc...) so that these rules and parameters can be be applied to different molecules more easily (by using the *import* command to load the file when needed).

```
# -- file "forcefield.lt" --

ForceField {

  # There are 2 atom types: "CA" and "R"
  write_once("Data Masses") {
    @atom:CA    13.0
    @atom:R     50.0
  }


  # Force-field parameters ("coeffs") go in the "In Settings" section:

  write_once("In Settings") {
    # Pairwise (non-bonded) interactions:
    #           atomType1 atomType2   epsilon sigma
    pair_coeff   @atom:CA @atom:CA      0.10 2.0
    pair_coeff   @atom:R  @atom:R       0.50 3.6
    # (Interactions between different atoms are determined by mixing rules.)
  }


  # 2-body (bonded) interactions:
  #
  #   Ubond(r) = k*(r-r0)^2
  #
  write_once("In Settings") {
    #             bond-type        k     r0
    bond_coeff  @bond:Sidechain   15.0   3.4
    bond_coeff  @bond:Backbone    15.0   3.7
  }


  # Although the simple "Monomer" object we defined above has only
  # two atoms, later on, we will create molecules with many bonds.
```

```
# By convention, in this file we keep track of all of the possible
# interactions which could exist between these atoms:


# Rules for determining 3-body (angle) interactions by atom and bond type:
# angle-type      atomType1 atomType2 atomType3  bondType1 bondType2

write_once("Data Angles By Type") {
  @angle:Backbone  @atom:CA  @atom:CA  @atom:CA   @bond:*   @bond:*
  @angle:Sidechain @atom:CA  @atom:CA  @atom:R    @bond:*   @bond:*
}


# Force-field parameters for 3-body (angle) interactions:
#
#   Uangle(theta) = k*(theta-theta0)^2
#
write_once("In Settings") {
  #            angle-type        k     theta0
  angle_coeff @angle:Backbone   30.00  114
  angle_coeff @angle:Sidechain  30.00  132
}


# 4-body interactions in this example are listed by atom type and (optionally)
# by bond type. (You can use wildcards * to accept all bond types.)
#
#   dihedralType atmType1 atmType2 atmType3 atmType4 bondType1 bType2 bType3
write_once("Data Dihedrals By Type") {
  @dihedral:CCCC @atom:CA @atom:CA @atom:CA @atom:CA  @bond:* @bond:* @bond:*
  @dihedral:RCCR @atom:R  @atom:CA @atom:CA @atom:R   @bond:* @bond:* @bond:*
}


# The forumula used in this example is:
#
# Udihedral(phi) = K * (1 + cos(n*phi - d))
#
#     The d parameter is in degrees, K is in kcal/mol/rad^2.
#
# The corresponding command is
# dihedral_coeff dihedralType      K  n   d  w(ignored)

write_once("In Settings") {
  dihedral_coeff @dihedral:CCCC   -0.5 1 -180 0.0
  dihedral_coeff @dihedral:RCCR   -1.5 1 -180 0.0
}


write_once("In Init") {
  # -- Styles used in "ForceField" --
  # -- (Changing these styles will change the formulas above) --
  units          real
```

```
    atom_style       full
    bond_style       harmonic
    angle_style      harmonic
    dihedral_style   charmm
    pair_style       lj/cut 11.0
  }
}
```

Any molecule that wants to access this information can use the "inherits ForceField" keyword. *(…as we did in the "monomer.lt" and "polymer.lt" files in theexample above. Note: the "import forcefield.lt" statement was also necessary because the information is located in a separate file: "forcefield.lt". You can customize these "By Type" rules further by altering the bond topology search rules and atom type symmetry. See appendix F.2 for details.)*

7.2   Wildcards

Star (*) and question mark (?) characters are multi and single-character wildcards. They can appear in any of the "pair_coeff", "bond_coeff", "angle_coeff", "dihedral_coeff", or "improper_coeff" commands. For example, the following excerpt tells moltemplate to assign nonbonded pair parameters "0.10 2.0" to *all* pairs of atoms whose atom type strings begin with the letter "C"

```
write_once("In Settings") {
  pair_coeff @atom:C* @atom:C* 0.10 2.0
}
```

Wildcards can also appear in any of the @atom or @bond type names in the "By Type" sections. The following rule will generate a dihedral angle interaction (of type "@angle:CCR") between any triplet of atoms if the last atom's type name ends with "R".

```
write_once("Data Angles By Type") {
  @angle:CCR @atom:* @atom:* @atom:*R
}
```

In this way, a small number of these rules can describe a large number of atom type combinations. Force fields like OPLSAA and COMPASS use this strategy to reduce the size of the entries in the "Angles By Type" section (and elsewhere). Note that rules with wildcards typically appear near the beginning of the "Data Angles By Type" section (and other "By Type" sections). Rules describing angles between specific atom type combinations should appear later in the list so that they can override the more general rules containing wildcards that appeared earlier.

  (Note: Regex based atom-type-name matching has been implemented, but this feature has not yet been tested. See section A.1. -Andrew 2020-8-09)

7.3 "Data Bonds By Type" and "Data Bond List"

It is also possible to determine *bond type* from *atom type*, by specifying a "Data Bonds By Type" section:

```
write_once("Data Bonds By Type") {
  @bond:Backbone  @atom:CA @atom:CA
  @bond:Sidechain @atom:CA  @atom:R
}
```

We can also put this information in the "ForceField" object. Later, in the "Monomer" and "Polymer" objects, we can omit the @bond types. For example, we could replace the "Data Bonds" section in the "Polymer" with a "Data Bond List" section:

```
write_once("Data Bond List") {
  $bond:backbone1  $atom:mon1/ca  $atom:mon2/ca
  $bond:backbone2  $atom:mon2/ca  $atom:mon3/ca
        :              :              :
}
```

Notice that we did not specify the "@bond:SideChain" and "@bond:Backbone" bond type information which would normally appear in the 2nd column of the "Data Bonds" section. While not very useful in this example, many all-atom force fields (eg. OPLSAA, GAFF, COMPASS) assign bond types by atom type. For this reason, molecules that use these force fields typically contain a "Data Bond List" section, instead of a "Data Bonds" section.

7.4 The *replace* command

The "replace" command is useful for people who want to publish their own custom force fields in moltemplate (LT) format. This command is typically used to simplify the names of atom types in modern force fields. In some force fields (eg, COMPASS, OPLSAA), atom type names are complicated by the the way they are used to lookup force field parameters. @atom type names can be quite long and difficult to type (such as "@atom:h1h_ph1h_bh1h_ah1_dh1_ih1"). The "replace" command allows *the people who use your force field* to refer to these atoms in their molecules with short names instead of long ones. Consider the following example:

```
replace{ @atom:C4  @atom:C4_aC4  }
replace{ @atom:H1  @atom:H1_aH1  }
replace{ @atom:C4o @atom:C4o_aC4 }
replace{ @atom:H1o @atom:H1o_aH1 }
```

In this example, "@atom:C4" and "@atom:H1" are shorthand referring to "@atom:C4_aC4" and "@atom:H1_aH1", respectively. *(The "replace" command works with all @-style variables, not just @atom type names. It does not work with $-style variables.)*

These longer atom names are often used in combination with "By Type" rules for generating angle and dihedral interactions. For example, consider a force field which uses the following rules for generating angle interactions:

```
write_once("Data Angles By Type") {
  @angle:HCH @atom:*_ah1 @atom:*_ac4 @atom:*_ah1
  @angle:CCH @atom:*_ac4 @atom:*_ac4 @atom:*_ah1
}
```

Through the use of wildcard characters (*), these two rules only depend on
the portion of the atom type name following the "_a" character ("h1", or
"c4"). Since multiple atom types share the same "h1" and "c4" name suf-
fixes, this significantly reduces the number of "Angles By Type" rules needed
for the carbon and hydrogen atoms in this example. (And this reduction
becomes even more dramatic as the number of atom types increases.)

The "replace" command is useful because it allows users to refer to
these long atoms by their short names ("@atom:C4" and "@atom:H1") when
creating molecules. For example:

```
# atom-id  mol-id atom-type charge   x         y         z
write("Data Atoms") {
  $atom:c  $mol:me @atom:C4  -0.18  0.0000  0.0000   0.0000
  $atom:h1 $mol:me @atom:H1   0.06  0.0000  0.6310   0.8924
  $atom:h2 $mol:me @atom:H1   0.06  0.0000  0.6310  -0.8924
  $atom:h3 $mol:me @atom:H1   0.06 -0.8924 -0.6310   0.0000
        :        :        :
}
```

7.5   "In Charges"

Recall that moltemplate was designed for simulating coarse grained molecu-
lar models. It's not uncommon for coarse grained models to use big particles
containing many atoms, whole proteins, or even larger complexes. It often
does not make sense to assign charge to particles in this size range, and
moltemplate does not force you to use a charge-bearing particle representa-
tion. But if you want to assign charges to particles, there are several ways
to do that.

Modern molecule-builder tools typically assign partial charges to atoms
using sophisticated ab initio physics-based calculations. Moltemplate does
not do this. However moltemplate does supports several optional methods
allowing you to assign particle charge according to atom type (@atom). For
example, here is an excerpt from the "loplsaa.lt" file (on 2020-8-09):

```
write_once("In Charges") {
  set type @atom:80L charge -0.222 # "Alkane CH3- (LOPLS)"
  set type @atom:81L charge -0.148 # "Alkane -CH2- (LOPLS)"
  :
}
```

This will set the charge of *all* atoms of type "@atom:80L" to -0.222, (re-
gardless of who they are bonded to).

Confusingly, the charge information is **not** written to the DATA file
created by moltemplate.sh. Instead the charges are written to a file whose
name ends in ".in.charges" (eg. "system.in.charges"). Later when you run

LAMMPS, you must remember to use the LAMMPS "include" command to load this file after you read the data file. For example:

```
read_data "system.data"
include "system.in.charges"
```

Note that any charge information specified in the "Data Atoms" section of your molecule (which ends up in "system.data") will be ignored. If you want to customize the charge of individual atoms in your molecule, add an "In Charges" section to the *end* of your molecule definition. For the carbon atoms in an alkane polymer (for example), you might use something like this:

```
write("In Charges") {
  set atom $atom:monomer[0]/c charge -0.222
  set atom $atom:monomer[1]/c charge -0.148
                 :
}
```

(For reference, the LAMMPS' "set" command is explained here: `https:// lammps. sandia. gov/ doc/ set. html`.)

7.6 "Data Charge By Bond"

The "Data Charge by Bond" section allows partial charges can be assigned to atoms according to the other atoms they are bonded to and their types. Here is a (slightly modified) excerpt from the "compass_published.lt" file:

```
write_once("Data Bonds By Type") {
  @atom:h1 @atom:si4        -0.1260 0.1260
  @atom:*bc4* @atom:*bsi4*  -0.1350 0.1350
}
```

Each bond between atoms contributes to the partial charge of those atoms. The first line tells moltemplate that any bond between atoms of type "@atom:h1" and "@atom:si4" modifies their charge by -0.1260 and 0.1260, respectively. The wildcard characters ("*") in the second line cause moltemplate to modify the partial charges of any bonded pair of atoms by -/+0.1350 if the first atom type contains the string "bc4" and the second atom type contains the string "bsi4". The final charge of each atom is determined by adding the contribution to its charge from each of the atoms it is bonded to.

Again, these charges will not be written to your DATA file. As explained above, after you load the DATA file, you must remember to use the LAMMPS "include" command to load the file containing the charge information. (For example: "include system.in.charges".) Again, if you need to, you can customize the charge of individual atoms in your molecule by placing an "write("In Charges")" section at the *end* of your molecule definition (as shown above).

7.7 The *force_fields* directory

Files containing popular force fields (like "oplsaa.lt" and "gaff2.lt") and molecule models (like "spce.lt") are stored in the "force_fields/" subdirectory distributed with moltemplate. (This directory is included when you download moltemplate using either git or pip.) You can load the contents of any of these files using the *import* statement. They do not need to be located in your local directory. You can add your own LT files there as well. This is a convenient way for many different examples to share the same force fields. If a shell environment variable named "TTREE_PATH" is defined, the directories listed there (delimited by ":") are also searched. *(Note: If a file you want to import can be found in multipl locations, the file in your local directory has priority.)*

8 Arrays, slices, and coordinate transformations

Moltemplate supports 1-dimensional, and multi-dimensional arrays. These can be used to create straight (or helical) polymers sheets, tubes, tori. They are also to fill solid 3-dimensional volumes with molecules or atoms. (See sections 4.2 and 8.6.)

Here we show an easier way to create the short polymer shown in section 6.1. You can make 7 copies of the *Monomer* molecule this way:

```
monomers = new Monomer[7]
```

This creates 7 new *Monomer* molecules (named *monomers[0]*, *monomers[1]*, *monomers[2]*, *monomers[3]*, ... *monomers[6]*). You can connect them with bonds in the same way we did earlier:

```
write("Data Bonds") {
  $bond:backbone1  @bond:Backbone  $atom:monomers[0]/ca  $atom:monomers[1]/ca
  $bond:backbone2  @bond:Backbone  $atom:monomers[1]/ca  $atom:monomers[2]/ca
  $bond:backbone3  @bond:Backbone  $atom:monomers[2]/ca  $atom:monomers[3]/ca
      :               :               :                     :
}
```

Unfortunately, by default, the coordinates of each molecule are identical. To prevent the atom coordinates from overlapping, you have several choices:

8.1 Transformations following brackets [] in a new statement

After every square-bracket [] in a new command, you can specify a list of transformations to apply. For example, we could have generated atomic coordinates for the the short polymer in section 6.1 using this command:

```
monomers = new Monomer [7].rot(180, 1,0,0).move(3.2,0,0)
```

This will create 7 molecules. The coordinates of the first molecule *monomers[0]* are will be unmodified. However each successive molecule will have its coordinates cumulatively modified by the commands "rot(180, 1,0,0)" followed by "move(3.2,0,0)".

optional: initial customizations (preceding [] brackets)

You can also make adjustments to the initial coordinates of the molecule before it is copied, and before any of the array transformations are applied. For example:

```
monomers = new Monomer.scale(1.5) [7].rot(180, 1,0,0).move(3.2,0,0)
```

In this example, the "scale(1.5)" transformation is applied once to enlarge every *Monomer* object initially. This will happen before any of the rotation and move commands are applied to build the polymer (so the 3.2 Angstrom spacings between each monomer will not be effected).

8.2 Transformations following instantiation

Alternately you apply transformations to a molecule after they have been created (even if they are part of an array).

```
monomers = new Monomer [7]

# Again, the first line creates the molecules named
# "monomers[0]", "monomers[1]", "monomers[2]", ... "monomers[6]".
# The following lines move them into position.
monomers[1].rot(180.0, 1,0,0).move(3.2,0,0)
monomers[2].rot(360.0, 1,0,0).move(6.4,0,0)
monomers[3].rot(540.0, 1,0,0).move(9.6,0,0)
monomers[4].rot(720.0, 1,0,0).move(12.8,0,0)
monomers[5].rot(900.0, 1,0,0).move(16.0,0,0)
monomers[6].rot(1080.0, 1,0,0).move(19.2,0,0)
```

8.3 Transformation order (general case)

A typical array of molecules might be instantiated this way:

```
mols = new Molecule.XFORMS1() [N].XFORMS2()
mols[*].XFORMS3()
```

The list of transformations denoted by "XFORMS1" in this example are applied to the molecule first. Then the transformations in "XFORMS2" are then applied to each copy of the molecule multiple times. (For the molecule with index "i", named "Molecule[i]", XFORMS2 will be applied i times.) Finally after all the molecules have been created, the list of transformations in XFORMS3 will be applied. For example, to create a ring of 10 polymers of radius 30.0, centered at position (0,25,0), use this notation:

```
polymer_ring = new Polymer.move(0,30,0) [10].rot(36,1,0,0)
  # After creating it, we can move the entire ring
  # (These commands are applied last.)
polymer_ring[*].move(0,25,0)
```
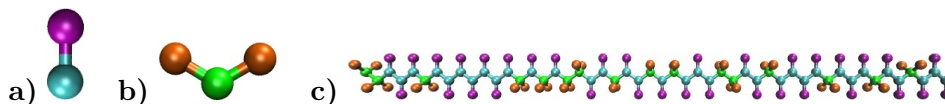
Figure 4: A random heteropolymer (**c**), composed of of *Monomer* and *Monomer3* monomer subunits (**a** and **b**) with (target) probabilities 0.6 and 0.4. (However, due to random fluctuations, the actual ratio in this case was 68% and 32%. To avoid this problem, see section 8.4.1.)

8.4 Random arrays

Arrays of random molecules can be generated using the *new random() []* syntax. For example, below we define a random polymer composed of 50 *Monomer* and *Monomer3* monomer subunits. (See figure 4.)

```
RandPoly50 inherits ForceField {
  # Make a chain of randomly chosen monomers:

  monomers = new random([Monomer, Monomer3], [0.6, 0.4], 123456)
                [50].rot(180,1,0,0).move(2.95, 0, 0)

  # Now, link the monomers together this way:
  write("Data Bonds") {
    $bond:bb1 @bond:Backbone $atom:monomers[0]/ca $atom:monomers[1]/ca
    $bond:bb2 @bond:Backbone $atom:monomers[1]/ca $atom:monomers[2]/ca
    $bond:bb3 @bond:Backbone $atom:monomers[2]/ca $atom:monomers[3]/ca
    $bond:bb4 @bond:Backbone $atom:monomers[3]/ca $atom:monomers[4]/ca

      ⋮

    $bond:bb50 @bond:Backbone $atom:monomers[48]/ca $atom:monomers[49]/ca
  }
  #(Note: Both the "Monomer" and "Monomer3" subunits contain atoms
  #       named "$atom:ca".
} #RandPoly50
```

It is also possible to fill a 2 or 3-dimensional volume with molecules randomly. This is discussed in section 8.8.

The *new random()* function takes 2 or 3 arguments: a list of molecule types (*Monomer* and *Monomer3* in this example), and a list of probabilities (*0.6* and *0.4*) both enclosed in square-brackets [].

8.4.1 Random arrays with exact molecule type counts

Recall that we requested that 60% of the molecules be of type "Monomer" and 40% type "Monomer3" (corresponding to 30 and 20, respectively). However, the resulting polymer (shown in figure 4) contains 34 "Monomer" and 16 "Monomer3" monomers (68% and 34%, respectively). This is because each time a monomer is created, a random number is generated to decide which type of monomer will be created. There is no guarantee that the total

final fraction of monomers will match the target probabilities exactly (60% and 40%, respectively). To specify the number of molecule types precisely, you can replace the list of probabilities "[0.6,0.4]" with a list of integers "[30,20]".

```
monomers = new random([Monomer, Monomer3], [30, 20], 123456)
                [50].rot(180,1,0,0).move(2.95, 0, 0)
```

This will create exactly 30 "Monomer" and 20 "Monomer3" monomers. (You can do this with multidimensional arrays as well. See section 8.9.1.)

Details regarding the *new random* command:

Note: You can tell moltemplate to customize the bond-types and angles, depending on the (types of) monomers are connected by each bond. The "random_heteropolymer" example downloadable at www.moltemplate.org demonstrates how to do this.

   Note: Although this example, there are only two monomer types ("Monomer" and "Monomer3"), there is no limit to the number of molecule types which appear in these lists (eg "[Monomer, Monomer3, 4bead],[0.2,0.3,0.2]")

   Note: An optional random-seed argument can also be included. (For example the *"123456"* shown above. If you omit this number, then you will get different results each time you run moltemplate.)

   Note: These lists can also contain vacancies/blanks. See section 8.9.)

   Note: Once a molecule containing random monomers is defined, (*"RandPoly50"* in this example), each copy of that molecule (created using the *new* command) is identical.

Optional: Customizing molecule positions in a *random()* array

You can customize the position of each type of molecule in the array, before the array is constructed. To do this, you can add additional movement commands after each molecule's type name in the list (eg "Monomer" and "Monomer3"):

```
monomers = new random([Monomer.move(0,0.01,0),
                       Monomer3.move(0,-0.01,0)],
                      [30,20],
                      123456)
                [50].rot(180,1,0,0).move(2.95, 0, 0)
```

The *.move(0,0.01,0)* and *.move(0,-0.01,0)* suffixes moves these monomers closer or further away from the polymer axis (the x axis in this example). This is not restricted to *.move()* commands. (You can also use *.rot()*, and *.scale()* commands as well.) These moves will be applied (in order from left to right), *before* any of the *.move()* and *.rot()* commands appearing later (following "[50]") are carried out.

8.5   [*] and [i-j] slice notation

You can move the entire array of molecules using "[*]" notation:

```
monomers[*].move(0,0,40)
```

(Note that "monomers.move(0,0,40)" does not work. You must include the "[*]".) You can also use range limits to move only some of the monomers:

```
monomers[2-4].move(0,0,40)
```

This will move only the third, fourth, and fifth monomers. If you are more familiar with python's slice notation, you can accomplish the same thing using:

```
monomers[2:5].move(0,0,40)
```

(In this case, the second integer (eg "5") is interpreted as a strict upper bound.)

(If these customizations are not enough for your needs, you can also always load atom coordinates from an external PDB or XYZ file. Such files can be generated by PACKMOL, or a variety of advanced graphical molecular modeling programs. For complex systems, this may be the best choice.)

8.5.1   Building arrays one interval at a time (using slice notation)

For a more complicated example, you can build polymers using slice notation. The example below demonstrates how to build a polymer, specifying which part is random, and and which part is not:

```
monomers[0]    = new Monomer3
monomers[1-48] = new random([Monomer, Monomer3], [30, 18], 123456)
                     [48].rot(180,1,0,0).move(2.95, 0, 0)
monomers[49]   = new Monomer3
# It's a good idea to move these monomers to keep them from overlapping
monomers[0].rot(180,1,0,0)
monomers[1-48].move(2.95,0,0)
monomers[49].move(144.55,0,0)    #(note: 144.55=49*2.95)
```

In this example, we insure that monomers[0] and monomers[49] are both of type "Monomer3" (while keeping the total number of "Monomer" and "Monomer3" monomers at 30 and 20, respectively).

*(Note: You can replace "monomers[1-48]" with "monomers[1:49]", or "monomers[1*48]", if you prefer that syntax style. You can build multidimensional arrays using slice notation as well, for example "molecules[3][10-19][4-6] = new Molecule[10][3]")*

8.6 Multidimensional arrays

The same techniques work with multidimensional arrays. Coordinate transformations can be applied to each layer in a multi-dimensional array. For example, to create a cubic lattice of 3x3x3 polymers: you would use this syntax:

```
molecules = new Polymer [3].move(30.0, 0, 0)
                        [3].move(0, 30.0, 0)
                        [3].move(0, 0, 30.0)
```

(Similar commands can be used with rotations to generate objects with cylindrical, helical, conical, or toroidal symmetry.)

8.7 Customizing individual rows, columns, or layers

Similarly, you can customize the position of individual polymers, or layers or columns using the methods above:

```
molecules[1][*][*].move(0,20,0)
molecules[*][1][*].move(0,0,20)
molecules[*][*][1].move(20,0,0)
```

See figure 3c) *(You can also use slice notation, eg "molecules[1][0-2][0-1].move(20,0,0)")*

You can delete part of an array and replace it with something else (eg *"Lipid"*) using slice notation:

```
delete molecules[0-1][1][1-2] # (shorthand for delete molecules[0][1][1]
                              #                delete molecules[0][1][2]
                              #                delete molecules[1][1][1]
                              #                delete molecules[1][1][2])


# Now replace the array elements we deleted:
molecules[0-1][1][1-2] = new Lipid [2].move(30,  0.0, 0.0)
                                   [2].move(0.0, 0.0, 30.0)


# ...and move them back to the location of the vacancies we created
molecules[0-1][1][1-2].move(0, 30.0, 30.0)
```

The word "Lipid" in this example is not important. It is the name of some other molecule type.

8.8 Creating random mixtures using multidimensional arrays

You can use *"new random()"* to fill space with a random mixture of molecules. The following 2-dimensional example creates a lipid bilayer (shown in figure 5) composed of an equal mixture of DPPC and DLPC lipids. (...Whose definition we omit here. See the online examples for details.)

```
import "lipids"                                    # define DPPC & DLPC
lipids = new random([DPPC,DLPC], [0.5,0.5], 123)   # "123"=random_seed
                  [19].move(7.5,     0,      0)     # lattice spacing 7.5
                  [22].move(3.75, 6.49519, 0)       # hexagonal lattice
                   [2].rot(180, 1, 0, 0)            # 2 monolayers
```


a)   b)
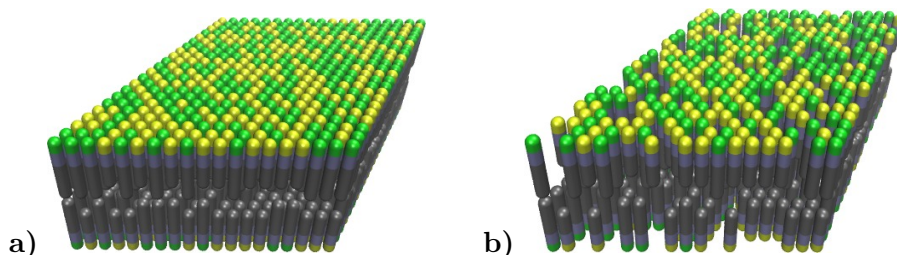
Figure 5:   A lipid bilayer membrane composed of a random equal mixture
of two different lipid types in a 1:1 ratio. (See section 8.8.) In **b)** one of the
molecule types was left blank leaving vacancies behind. (See section 8.9.)

8.9   Inserting random vacancies

The list of molecule types passed to the *random()* function may contain
blanks. In the next example, 30% of the lipids are missing:

```
lipids = new random([DPPC, ,DLPC], [0.35,0.3,0.35], 123) # 2nd element is blank
                  [19].move(7.5,     0,      0)
                  [22].move(3.75, 6.49519, 0)
                   [2].rot(180, 1, 0, 0)
```

The results are shown in figure 5b). *(Note: When this happens, the ar-
ray will contain missing elements. Any attempt to access the atoms inside
these missing molecules will generate an error message, however moving or
deleting array entries using [*] or [i-j] notation should be safe.)*

8.9.1   Random multidimensional arrays with exact type counts

Due to random fluctuations the number of DPPC and DLPC lipids created
may not equal exactly $0.35 \times$ of the number of entries in the array,

Alternately, you can specify the exact number of DPPC and DLPC
molecules you desire (as opposed to a list of probabilities). To do this,
replace the list of probabilities with integers:

```
lipids = new random([DPPC, ,DLPC], [293,250,293], 123)
                  [19].move(7.5,     0,      0)
                  [22].move(3.75, 6.49519, 0)
                   [2].rot(180, 1, 0, 0)
```

This will generate exactly 293 DPPC and DLPC molecules (and 250 *blank*
entries, since the second molecule type was unspecified). The sum (ie
293+250+293) must equal the number of entries in the array you are creat-
ing (ie 19x22x2).

8.10 Cutting rectangular holes using delete

The delete command can be used to cut large holes in 1, 2, and 3-dimensional objects. For example, consider a simple 3-dimensional 12x12x12 cube of molecules. (For simplicity, each "molecule" in this example contains only one atom. These atoms appear as blue spheres in figure 6.)

```
molecules = new OneAtomMolecule [12].move(3.0,0,0)
                                [12].move(0,3.0,0)
                                [12].move(0,0,3.0)
```

Then, we cut out some rectangular vacancies:

```
delete molecules[*][*][2]
delete molecules[*][*][8]
delete molecules[6-7][0-8][5-6]
```

The result of these operations is shown in figure 6. *(Note: You may move or delete previously deleted array elements more than once, and/or deleting overlapping rectangular regions without error.)*
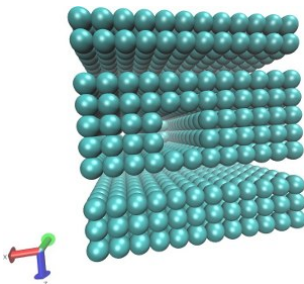
Figure 6: Rectangular holes can be carved out of an array of molecules (represented here by blue spheres) using the "delete" command. Three delete commands were used to remove the two planar regions and the rectangular hole in the center.

9 Customizing molecule position and topology

By default, each copy of a molecule created using the *new* command is identical. This need not be the case.

As discussed in section 8.2, individual molecules which were recently created can be moved, rotated, and scaled. You can also overwrite or delete individual atoms, bonds, and other interactions within a molecule, or their subunits. (See sections 9.3.2, 9.1.1, 9.1.2, and 9.2.) You make any of these modifications to *some* copies of the molecule without effecting other copies. Furthermore, if those molecules are compound objects (if they contain individual molecular subunits within them), then you can rearrange the positions of their subunits as well. And all of this can be done from anywhere else in the LT file.

For example, suppose we used the "Polymer" molecule we defined above to create a larger, more complicated "MolecularComplex" molecule.

```
MolecularComplex inherits ForceField {
  polymers[0] = new Polymer
  polymers[1] = new Polymer.rot(180,1,0,0).move(0, 12.4, 0)
}
mol_complex = new MolecularComplex
```

The *MolecularComplex* molecule is shown in figure 7a). *Optional: If you want all the atoms in a "MolecularComplex" to share the same molecule-ID, then define "MolecularComplex" this way:*

```
MolecularComplex inherits ForceField {
  create_var { $mol }
  polymers[0] = new Polymer
  polymers[1] = new Polymer.rot(180,1,0,0).move(0, 12.4, 0)
}
```

For this to work, you must also delete the "create_var {$mol}" line from the definition of the Polymer molecule. See section 6.1.
    We can subsequently customize the position of the 3rd monomer ("monomers[2]") of the second polymer ("polymers[1]"), this way:

```
mol_complex/polymers[1]/monomers[2].move(0,0.2,0.6)
```

    This does not effect the position of *monomers[2]* in *polymers[0]*. (or in any other *"Polymer"* or *"MolecularComplex"* molecule.) If you want to do the same thing for both polymers, you could use a wildcard character "*"

```
mol_complex/polymers[*]/monomers[2].move(0,0.2,0.6)
```

If you want to move both polymers, you can use:

```
mol_complex/polymers[*].move(0,0.2,0.6)
```

you could use a wildcard character "*" (You can also use ranged (slice) notation, such as "polymers[0-1]", as an alternative to "polymers[*]". See section 8.5.
    To make changes that apply to every subsequently created *"Polymer"* or *"MolecularComplex"* molecule, see section 9.4.)

9.1 Customizing individual atoms or bonds

9.1.1 Customizing individual atom locations

The "move" or "rot" commands can not be used to control the positions of *individual atoms.* Instead simply overwrite their coordinates this way:

```
write("Data Atoms") {
  $atom:mol_complex/polymers[0]/monomers[2]/ca $mol:mol_complex @atom:R 0 6.4 8.2 0.6
}
```

This is an case where we must use the *full* variable name of the atom ("$atom:mol_complex/polymers[0]/monomers[2]/ca") to indicate *which* "ca" atom we want to overwrite (In this case, we want to modify the "ca" atom belonging to "monomers[2]" in "polymers[0]" in "mol_complex").

9.1.2 Customizing individual bonds, angles, dihedrals,...

Similarly, you can customize existing bonds, angles, etc... by overwriting the line containing a reference to that particular bond (or angle, ...). For example, you can increase the rest length of the spring representing the 3rd backbone bond in the first polymer, by changing it from type "@bond:Backbone" to "@bond:LongBond"

```
write("Data Bonds") {
  $bond:mol_complex/polymers[0]/backbone3 @bond:ForceField/LongBond &
      $atom:mol_complex/polymers[0]/monomers[2]/ca &
      $atom:mol_complex/polymers[0]/monomers[3]/ca
}
```

Note: The optional "&" character is used in LAMMPS to split a long command into multiple lines. This command is quite long since we are outside the definition of the polymer molecule, and we must provide the full-path for every variable (for example "mol_complex/polymers[0]", and "ForceField").

Alternatively, if you prefer, you can *delete* the bond and define a new bond connecting the same pair of atoms (see section 9.3).

Of course, at some point you must also create a new "bond_coeff" command defining the properties of this new type of bond (for example to increase the length of the new spring). You can either edit the "forcefield.lt" file, *or* simply add the following lines of text somewhere in one of your .LT files (for example "system.lt")

```
# Note: This will augment the "ForceField" object, not overwrite it:
ForceField {
  write_once("In Settings") {
    #                new bond-type   k     r0
    bond_coeff  @bond:LongBond   10.0  4.8
  }
}
```

9.2 Adding bonds and angles to individual molecules

Adding additional bonds within a molecule can be accomplished by writing additional lines of text to the "Data Bonds" section. (This is what we did when we added bonds between monomers to create a polymer in section 6.1.) Again, bonds and atom names must be referred to by their *full* names. Bonds and bonded interactions can be deleted using the "delete" command. (See section 9.3.)

9.3 The delete command

9.3.1 Deleting molecules or molecular subunits

Molecules can be further customized by deleting individual atoms, bonds, bonded-interactions, and entire subunits. We can **delete** the 3rd monomer of the second polymer, use the "delete" command:

```
delete mol_complex/polymers[1]/monomers[2]
```

9.3.2 Deleting atoms, bonds, angles, dihedrals, and impropers

Individual atoms or bonds can be deleted in a similar way:

```
delete mol_complex/polymers[1]/monomers[3]/ca   #<-- deletes the "ca" atom
delete mol_complex/polymers[1]/monomers[4]/cr   #<-- deletes the "cr" bond
```

Whenever an atom or a molecule is deleted, the bonds, angles, dihedrals, and improper interactions involving those atoms are deleted as well. *Note: You must omit the "$" character when deleting atoms, bonds, or angles, as we did in the two lines above).*

When a bond is deleted, any angular, dihedral, or improper interactions which were *automatically* generated by moltemplate are removed as well. (However other bonded interactions explicitly listed by the user in their "Data Angles", "Data Dihedrals", or "Data Impropers" sections are not removed. These need to be deleted manually.)

Multiple molecules can moved or deleted in a single command. For example, the following command deletes the third, fourth, and fifth monomers from both polymers[0] and polymers[1]:

```
delete mol_complex/polymers[*]/monomers[2-4]
```

See section 8.5 for an explanation of ranged ("[2-4]") array notation, and wildcard characters ("*").

Minor bug notice: Deleting atoms or molecules may cause inaccuracies in the $atoms, $bonds, $angles, $dihedrals, and $impropers sections of the "ttree_assignments.txt" file. (If this is a problem, please email me. -Andrew 2019-9-03.) Fortunately, this should not harm the resulting LAMMPS data files or input scripts generated by moltemplate. They should still work with LAMMPS.

*WARNING: The **delete** feature is experimental. There have been a few bugs in the **delete** command, but by 2019-9-03 these should be fixed. Please report any problems you find. As always, be sure to visualize your structures to make sure they look reasonable. (…by running moltemplate.sh using the "-vmd" command line option, for example. See sections 4.3, C for details.)*

9.4 Customizing molecule *types*

You can create modified versions of existing molecule *types*, without having to redefine the entire molecule. For example:

```
MolecularComplex0 = MolecularComplex.move(-9.6,-6.2, 0).scale(0.3125)
```

or equivalently:

```
MolecularComplex0 = MolecularComplex
MolecularComplex0.move(-9.6,-6.2, 0).scale(0.3125)
```

This creates a new type of molecule named "MolecularComplex0" whose coordinates have been centered and rescaled. (Note that the "scale()" command only effects the atomic coordinates. (You will have to override earlier force field settings, such as atomic radii and bond-lengths in order for this to work properly.) If we want to make additional customizations (such as adding atoms, bonds, or molecular subunits), we could use this syntax:

```
MolecularComplex0 = MolecularComplex

# Add some new atoms connecting the two polymers in the mol_complex

MolecularComplex0 inherits ForceField {
  write("Data Atoms") {
    $atom:t1 $mol:... @atom:CA   0.0    23.0    0.0     0.0
    $atom:t2 $mol:... @atom:CA   0.0    24.7    4.0     0.0
    $atom:t3 $mol:... @atom:CA   0.0    24.7    8.4     0.0
    $atom:t4 $mol:... @atom:CA   0.0    23.0    12.4    0.0
  }

  write("Data Bonds") {
    $bond:b1 @bond:Backbone $atom:polymers[0]/res7/CA $atom:t1
    $bond:b2 @bond:Backbone $atom:t1 $atom:t2
    $bond:b3 @bond:Backbone $atom:t2 $atom:t3
    $bond:b4 @bond:Backbone $atom:t3 $atom:t4
    $bond:b5 @bond:Backbone $atom:t4 $atom:polymers[1]/res7/ca
  }
}

# Center and rescale the atoms in all "MolecularComplex0"
MolecularComplex0.move(-9.6,-6.2, 0).scale(0.3125)
```

The result of these modifications is shown in figure 7b).

a) b)
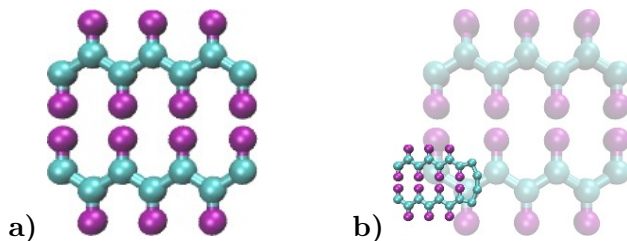
Figure 7: **a)** The "MolecularComplex" molecule. This is a contrived example consisting of two "Polymers". See section 6.1 **b)** A customized version of the "MolecularComplex" molecule. (The original "MolecularComplex" is shown faded in the background for comparison.)

*Note: These coordinate transformations will be applied **after** the molecule is constructed. (If you add atoms to the molecule, these will be added before the coordinate transformations are applied, even if you issue the command later.) Consequently, to make things clear, I recommend placing the coordinate transforms applied to an entire molecule type **after** all of its internal details (bonds, atoms, subunits) have been declared, as we did here.*

(Advanced) Inheritance

The *MolecularComplex0* molecule is a type of *MolecularComplex* molecule. For those who are familiar with programming, relationships like this are

analogous to the relationship between parent and child objects in an object-oriented programming language. More general kinds of inheritance are supported by moltemplate and are discussed in section 10.7.

(Advanced) Multiple Inheritance

If we wanted, we could have created a new molecule type (like *"Molecular-Complex0"*) which includes atom types and features from *multiple* different types of molecules. Section 10.7 mentions one way to do this and section 10.7.3 discusses alternate approaches.

10   Advanced moltemplate usage

This chapter includes a more detailed discussion of moltemplate syntax. The goal of this chapter is to help you write moltemplate (".LT") files in a *portable* way, so that they can be shared with others. The ".LT" format is a flexible file format for storing both molecules and force field parameters in LAMMPS. There are a variety of ways to do this. For completeness, this chapter includes a discussion of these different methods, and a comparison between them. However, when using force fields, most users are encouraged to follow the syntax explained in chapters 10.7 and 7.

10.1   Mixing molecule types

In section 4.1, we provided an example of an SPCE water molecule model. This example was simple to understand. But LAMMPS has the ability to combine molecules using different kinds of force-fields together in the same simulation. If you want to share your ".LT" file with others, it's not safe to assume that all interactions use the same simple harmonic bond or angle styles that we used in that example. For example, we used harmonic restoring forces to preserve the water angle at $109.47°$, but other users may want to mix this SPCE water with a small number of molecules which use a more complicated angular potential formula, or tabular angle potentials. Using the "hybrid" keyword, you can avoid this limitation. A more robust example using "hybrid" styles is included below.

```
# file "spce.lt"
#
#    h1     h2
#      \   /
#        o

SPCE {

  write_once("In Init") {
    # -- Default styles (for solo "SPCE" water) --
    units        real
    atom_style   full
    pair_style   hybrid lj/charmm/coul/long 9.0 10.0 10.0
```

```
    bond_style   hybrid harmonic
    angle_style  hybrid harmonic
    kspace_style pppm 0.0001
    pair_modify  mix arithmetic
}


# AtomID   MolID  AtomType  charge  coordX    coordY    coordZ
write("Data Atoms") {
  $atom:o  $mol:w @atom:O -0.8476  0.0000000 0.00000 0.000000
  $atom:h1 $mol:w @atom:H  0.4238  0.8164904 0.00000  0.5773590
  $atom:h2 $mol:w @atom:H  0.4238  -0.8164904 0.00000 0.5773590
}


# atom-type  Mass
write_once("Data Masses") {
  @atom:O     15.9994
  @atom:H      1.008
}


# -- Forces between atoms (non-bonded) --


#           atomTypeI atomTypeJ    pair-style-name     parameter-list
write("In Settings") {
  pair_coeff   @atom:O @atom:O  lj/charmm/coul/long   0.1553  3.166
  pair_coeff   @atom:H @atom:H  lj/charmm/coul/long   0.0      2.058
}


# -- Forces between atoms (bonded) --


#  bond-id   bond-type   atom-id1 atom-id2
write("Data Bonds") {
  $bond:oh1  @bond:OH   $atom:o  $atom:h1
  $bond:oh2  @bond:OH   $atom:o  $atom:h2
}


#              bond-type   bond-style-name  parameter-list
write("In Settings") {
  bond_coeff   @bond:OH      harmonic       200.0   1.0
}


# angle-id    angle-type   atom-id1 atom-id2 atom-id3
write("Data Angles") {
  $angle:hoh @angle:HOH  $atom:h1 $atom:o $atom:h2
}


#              angle-type  angle-style-name  parameter-list
write("In Settings) {
  angle_coeff  @angle:HOH     harmonic         200.0   109.47
```

```
  }

  # miscellaneous
  write_once("In Settings") {
    group spce type  @atom:O  @atom:H
    fix fRATTLE spce rattle 0.0001 10 100 b @bond:OH a @angle:HOH
    # (Remember to "unfix" fRATTLE during minimization.)
  }

} # SPCE
```

There are two differences between this molecule definition and the "spce_simple.lt" example from section 4.1:

Hybrid force field styles

To experienced LAMMPS users, it may seem strange that in this example that we have chosen "hybrid" styles followed by only one force-field style ("harmonic"). However this will make your molecule easier to share with others. When other people use your LT file, they can override these styles as explained in section 10.2.

10.2   Combining molecules with different force field styles

Later on, if a user wants to combine the SPCE water molecule with another molecule which uses a tabular pair_style (for example), they would have to specify the complete hybrid pair_style in the "Init" section of their LT file. For example:

```
import "spce.lt"
import "other_molecule.lt"

write_once("In Init") {
  pair_style hybrid lj/charmm/coul/long 9 10 10 table spline 1000
}
```

Note: By placing the "write_once("In Init"){ }" statement *after* "import "spce.lt"", this insures that the pair_style commands issued here will override the pair_style commands issued earlier "spce.lt". This allows moltemplate users users to combine their molecules "spce.lt" file shown here with other template files without modification (assuming the atom styles match).

Warning: Force-field parameters belong in "In Settings", not "Data"

LAMMPS allows users to store force-field parameters ("Coeffs") in two places: a DATA file, *or* an INPUT script. Similarly, moltemplate technicaly allows you to store these parameters in in the "Data" sections of your .LT file:

> write_once("Data Pair Coeffs")
>
> write_once("Data Bond Coeffs")

write_once("Data Angle Coeffs")

write_once("Data Dihedral Coeffs")

write_once("Data Improper Coeffs")

However, for portability reasons, this is discouraged. Instead, declare your force field parameters as we do in this manual, using the corresponding input script commands. (For example, "pair_coeff", "bond_coeff", "angle_coeff", "dihedral_coeff", and "improper_coeff" commands. As in the examples, these commands usually should be located in the "write_once("In Settings")" sections of your .LT files.)

10.3   Nesting

Molecule names such as "Solvent" (or even "Water") are short and easy to type, but are vague and are not portable. If you use common, generic molecule names, you will not be able to combine your molecule templates with templates written by others (without carefully checking for naming conflicts). LT files were meant to be used for storing and exchanging libraries of different molecule types.

Suppose, for example, that you want to run a simulation consisting of different molecule types, each of which belong to different LT files. Suppose two of the LT files both happen to contain definitions for "Water". Moltemplate does not detect these name clashes automatically and instead attempts to merge the two versions of "Water" together, (most likely creating a molecule with 6 atoms instead of 3). This is presumably not what you want.

As the number of molecule types grows, the possibility of naming clashes increases. As the behavior of the same molecule can be approximated using many different force fields, one has to be careful to avoid clashing molecule names.

To alleviate the problem, you can "nest" your molecules inside the definition of other molecules or namespace objects. This reduces the scope in which your molecule is defined. See section 10.5 for an example.

10.4   A simple force-field example

Force-field parameters can be shared by groups of related molecules. In the example below, we create an object named "TraPPE". Later we use it to define a new molecule named "Cyclopentane".

The following example defines a coarse-grained (united-atom) version of a "cyclopentane" molecule. (Hydrogen atoms have been omitted.) In this example, only the atom types (and positions) and the bonds connecting them need to be specified. The interactions between them are determined automatically by the settings in the force-field file "trappe1998.lt".

```
import "trappe1998.lt"
```

```
cyclopentane {

  # AtomID  MolID('.'=this) AtomType  charge coordX  coordY   coordZ
  write("Data Atoms") {
    $atom:c1 $mol:cp @atom:TraPPE/CH2 0.0 0.0000 0.000000000 1.0000000
    $atom:c2 $mol:cp @atom:TraPPE/CH2 0.0 0.0000 0.951056516 0.3090170
    $atom:c3 $mol:cp @atom:TraPPE/CH2 0.0 0.0000 0.587785252 -0.809017
    $atom:c4 $mol:cp @atom:TraPPE/CH2 0.0 0.0000 -0.587785252 -0.809017
    $atom:c5 $mol:cp @atom:TraPPE/CH2 0.0 0.0000 -0.951056516 0.3090170
  }


  write("Data Bonds") {
    $bond:bond1 @bond:TraPPE/CC $atom:c1 $atom:c2
    $bond:bond2 @bond:TraPPE/CC $atom:c2 $atom:c3
    $bond:bond3 @bond:TraPPE/CC $atom:c3 $atom:c4
    $bond:bond4 @bond:TraPPE/CC $atom:c4 $atom:c5
    $bond:bond5 @bond:TraPPE/CC $atom:c5 $atom:c1
  }
}
```

(The "TraPPE/" notation is explained below.)

NOTE: While conceptually simple, this is not currently the recommended way to use force fields in moltemplate. *(See section 10.7 for a better way.)*

...Then we can create copies of this molecule in the same way we did with SPCE:

```
# A cubic lattice of 125 cyclopentane molecules (12-angstrom spacing)
mols = new Cyclopentane [5].move(0,0,12) [5].move(0,12,0) [5].move(12,0,0)
```

Unlike the SPCE example, we don't have to specify all of the interactions between these atoms because the atom and bond types (CH2, CC). match the type-names defined in the "trappe1998.lt" file. This file contains a collection of atom types and force-field parameters for coarse-grained hydrocarbon chains. (See [8] for details.) This way, the "CH2" atoms in cyclopentane will interact with, and behave identically to any "CH2" atom from any other molecule which uses the TraPPE force field. (The same is true for other atom types, and interaction-types which are specific to "TraPPE", such as "@atom:TraPPE/CH3", "@bond:TraPPE/CC", etc... Another molecule which uses the TraPPE force field is discussed later in section 10.5.) The important parts of the "trappe1998.lt" file are shown below:

10.4.1 Namespace example

```
# -- file "trappe1998.lt" --

TraPPE {
  write_once("Data Masses") {
    @atom:CH2 14.1707
    @atom:CH3 15.2507
```

55

```
  }
  write_once("In Settings") {
    bond_coeff    @bond:CC     harmonic   120.0   1.54
    angle_coeff   @angle:CCC   harmonic   62.0022 114
    dihedral_coeff @dihedral:CCCC opls 1.411036 -0.271016 3.145034 0.0
    pair_coeff @atom:CH2 @atom:CH2 lj/charmm/coul/charmm 0.091411522 3.95
    pair_coeff @atom:CH3 @atom:CH3 lj/charmm/coul/charmm 0.194746286 3.75
    # (Interactions between different atom types use mixing rules.)
    # (Hybrid styles were used for portability.)
  }
  write_once("Data Angles By Type") {
    @angle:CCC @atom:C* @atom:C* @atom:C* @bond:CC @bond:CC
  }
  write_once("Data Dihedrals By Type") {
   @dihedral:CCCC @atom:C* @atom:C* @atom:C* @atom:C* @bond:CC @bond:CC @bond:CC
  }
}
```

In addition to the atom-type names and masses, this file stores the force-field parameters (coeffs) for the interactions between them.

Bonded interactions *by type*

Again, the "Data Angles By Type" and "Data Dihedrals By Type" sections tell moltemplate.sh that bonded 3-body and 4-body interactions exist between any 3 or 4 consecutively bonded carbon atoms (of type CH2, CH3, or CH4) assuming they are bonded using "CC" (saturated) bonds. The "*" character is a wild-card. "C*" matches "CH2", "CH3", and "CH4". (Bond-types can be omitted or replaced with wild-cards "@bond:*".)

Namespaces and nesting:

Names like "CH2" and "CC" are extremely common. To avoid confusing them with similarly named atoms and bonds in other molecules, we enclose them ("nest" them) within a *namespace* ("TraPPE", in this example). Unlike "SPCE" and "Cyclopentane", "TraPPE" is not a molecule. It is just a container of atom types, bond-types and force-field parameters shared by other molecules. We do this to distinguish them from other atoms and bonds which have the same name, but mean something else. Elsewhere we can refer to these atom/bond types as "@atom:TraPPE/CH2" and "@bond:TraPPE/CC". (You can also avoid repeating the cumbersome "TraPPE/" prefix for molecules defined within the TraPPE namespace. For example, see section 10.5.)

10.5   Nested molecules

Earlier in section 10.4.1, we created an object named "TraPPE" and used it to create a molecule named "Cyclopentane". Here we use it to demonstrate

nesting. Suppose we define a new molecule "Butane" consisting of 4 coarse-grained (united-atom) carbon-like beads, whose types are named "CH2" and "CH3".

```
# -- file "trappe_butane.lt" --

import "trappe1998.lt"

Butane {
  write("Data Atoms"){
    $atom:c1 $mol:bt @atom:TraPPE/CH3 0.0   0.419372   0.000 -1.937329
    $atom:c2 $mol:bt @atom:TraPPE/CH2 0.0  -0.419372   0.000 -0.645776
    $atom:c3 $mol:bt @atom:TraPPE/CH2 0.0   0.419372   0.000  0.645776
    $atom:c4 $mol:bt @atom:TraPPE/CH3 0.0  -0.419372   0.0000 1.937329
  }
  write("Data Bonds"){
    $bond:b1 @bond:TraPPE/CC $atom:c1 $atom:c2
    $bond:b2 @bond:TraPPE/CC $atom:c2 $atom:c3
    $bond:b3 @bond:TraPPE/CC $atom:c3 $atom:c4
  }
}
```

NOTE: Again, this is not the recommended way to use force fields. *(See section 10.7 for a cleaner, simpler way.)*

As mentioned above, it may be simpler to nest our "Butane" within "TraPPE", so that so that it does not get confused with other (perhaps all-atom) representations of the butane molecule. In that case, we would use:

```
# -- file "trappe_butane.lt" --

import "trappe1998.lt"

TraPPE {
  Butane {
    write("Data Atoms"){
      $atom:c1 $mol:bt @atom:../CH3 0.0   0.419372   0.000 -1.937329
      $atom:c2 $mol:bt @atom:../CH2 0.0  -0.419372   0.000 -0.645776
      $atom:c3 $mol:bt @atom:../CH2 0.0   0.419372   0.000  0.645776
      $atom:c4 $mol:bt @atom:../CH3 0.0  -0.419372   0.0000 1.937329
    }
    write("Data Bonds"){
      $bond:b1 @bond:../CC $atom:c1 $atom:c2
      $bond:b2 @bond:../CC $atom:c2 $atom:c3
      $bond:b3 @bond:../CC $atom:c3 $atom:c4
    }
  }
}
```

NOTE: Again, although the "nesting" method explained here works, a simpler, better way to use force fields is demonstrated in section 10.7.

Also note that wrapping Butane within "TraPPE{ }" clause merely appends additional content to be added to the "TraPPE" object defined in the "trappe1998.lt" file (which was included earlier). It does not overwrite it. Again "../" tells moltemplate use the "CH2" atom defined in the context of the TraPPE environment (IE. one level up). This insures that moltemplate does not create a new "CH2" atom type which is local to the Butane molecule. (Again, by default all atom types and other variables are local. See section 5.2.5.)

To use this butane molecule in a simulation, you would import the file containing the butane definition, and use a "new" command to create one or more butane molecules.

```
import "trappe_butane.lt"
new butane = TraPPE/Butane
```

(You don't need to import "trappe1998.lt" in this example because it was imported within "trappe_butane.lt".) The "TraPPE/" prefix before "Butane" lets moltemplate/ttree know that butane was defined *locally* within TraPPE.

Note: An alternative procedure using **inheritance** *exists which may be a cleaner way to handle these kinds of relationships. See sections 10.7 and 10.7.1.*

10.6   Path syntax: "../", ".../", and "$mol:."

Generally, multiple slashes ("/") as well as ("../") can be used build a path that indicates the (relative) location of any other molecule in the object hierarchy. (The ".", "/" and ".." symbols are used here in the same way they are used to specify a path in a unix-like file-system. For example, the "." in "$mol:." refers to the current molecule (instance), in the same way that "./" refers to the current directory. (Note: *"$mol"* is shorthand for *"$mol:."*)

A slash by itself, "/", refers to the *global environment.* This is the outermost environment in which all molecules are defined/created.

10.6.1   *(Advanced)* Ellipsis notation ".../"

If you are using multiple levels of nesting, and if you don't know (or if you don't want to specify) where a particular molecule type or atom type (such as "CH2") was defined, you can refer to it using ".../CH2" instead of "../CH2". The "..." ellipsis syntax searches up the tree of nested molecules to find the target (the text following the "/" slash).

10.6.2   *(Advanced)* $mol:... notation

Recall that LAMMPS allows users the option to assign *molecule-IDs* to each atom. (In the water example (section 4.1), atoms in each water molecule

is assigned to a molecule-ID, denoted "$mol:w". In that example, the "w" was the name given to that molecule's ID.)

   If you want to build large molecules using smaller pieces as building-blocks moltemplate has a way to allow all the the atoms to share the same molecule-ID. To refer to the ID of the molecule to which you belong, use "$mol:...". (If none of the molecule-objects which instantiate the current molecule-object define a variable in the $mol category, then a new local $mol variable will be created automatically.) This means that the second column of each line of the "Data Atoms" section should contain "$mol:..." (assuming "atom_style full" or "molecular" is used).

   The "..." syntax is explained in section 6.1, and more formally in section 10.6, and appendix G.1

10.7   Inheritance

We could have defined *Butane* this way:

```
import "trappe1998.lt"

Butane inherits TraPPE {
  write("Data Atoms"){
    $atom:c1 $mol:bt @atom:CH3 0.0  0.419372  0.000 -1.937329
    $atom:c2 $mol:bt @atom:CH2 0.0  -0.419372  0.000 -0.645776
    $atom:c3 $mol:bt @atom:CH2 0.0  0.419372  0.000  0.645776
    $atom:c4 $mol:bt @atom:CH3 0.0  -0.419372  0.0000 1.937329
  }
  write("Data Bonds"){
    $bond:b1 @bond:CC $atom:c1 $atom:c2
    $bond:b2 @bond:CC $atom:c2 $atom:c3
    $bond:b3 @bond:CC $atom:c3 $atom:c4
  }
}
```

The "inherits" keyword causes *Butane* to have all of the attributes (such as atom types, bond types, molecule definitions) of the "parent" object (*TraPPE*). Defining *Butane* this way means that you can directly access these molecule types, atom types, and bond types. You can refer to the CH3 atom type "@atom:CH3" instead of "@atom:TraPPE/CH3", or "@atom:../CH3" for example. (Eliminating unnecessary redundant text, like "TraPPE/" and "../", reduces the chance of typos or spelling errors.) **This is the preferred way to use force fields in moltemplate.**

10.7.1   Multiple inheritance:

A molecule can inherit from multiple parents. This is one way you can allow the *Butane* molecule to borrow atom, bond, angle, dihedral, and improper types from *multiple* different force-field parents:

```
import "trappe1998.lt"
import "oplsaa.lt"
```

```
Butane inherits TraPPE OPLSAA {
  ...
}
```

Details:Moltemplate attempts to resolve duplicate atom types or molecule types if they are found in both parents, giving priority to the first parent in the list of parents following the "inherits" keyword. ("TraPPE" in this example.)

10.7.2   Inheritance *vs.* Nesting

If two molecules are related to each other this way: *"A is a particular type of B"*, then consider using inheritance instead of nesting (or object composition). In this example (with *Butane* and *TraPPE*) either nesting or inheritance would work (but inheritance is a little bit cleaner and safer).

   Again, one very minor advantage to nesting *Butane* inside *TraPPE*, is that it prevents the name *Butane* from being confused with or conflicting with any other versions of the *Butane* molecule defined elsewhere. (Usually this is not a consideration.)

10.7.3   Inheritance *vs.* Object Composition

On the other hand, if two molecules are related to each other this way: *"A is comprised of B and C"*, then you might consider using object composition instead of inheritance. For example:

```
import "B.lt"  # <-- defines the molecule type "B"

import "C.lt"  # <-- defines the molecule type "C"

A {
  b = new B
  c = new C
}
```

11   Known bugs and limitations

Please report any bugs you find by email to **jewett.aij@gmail.com**, or to the lammps-users mailing list.

   1) LAMMPS-style molecule-templates are *not* supported. The DATA files created by moltemplate are not in the correct format to be read by the LAMMPS *molecule* command. (This is because this command was added after moltemplate was written.) However the formats are similar, and the relevant information can be extracted using a text-editor and converted to the other format. (Using a text-editor and awk, or a spreadsheet program. For more information on these file formats, `http://lammps.sandia.gov/doc/read_data.html http://lammps.sandia.gov/doc/molecule.html`.) Again,

feel free to contact **jewett.aij@gmail.com** to request support for LAMMPS-style molecule templates.

2) Moltemplate consumes a large amount of memory (RAM)

Memory use grows proportional to system size. As of 2019-9-03, setting up a system of 1000000 atoms using moltemplate currently requires between 2.7 and 12 GB of *available* memory. (Systems with many bonds and angles consume more memory, as well as systems with a high molecule count.) Unfortunately this code was not carefully written to minimize memory usage. (In addition, python programs can require more than 10 times as much memory as similar programs written in C/C++.)

This problem might be alleviated by using other python interpreters with a lower memory footprint. Alternately, it may be necessary to split a large system into pieces, run moltemplate on each piece, and combine the resulting data files into one large data file later.

Also, computers with a moderate amount of RAM can be rented very cheaply. (For example, see `https://cloud.google.com/compute/`.)

When setting up large simulations with moltemplate, consider using the "ulimit" command to prevent system crashes. (If you are on a shared computer, ask an administrator to do this.) If these options are not available, you can always run a resource monitor (like "top") before starting moltemplate and kill the process if it's memory usage exceeds 80%.

3) Limited support for non-point-like atoms:

As of 2019-9-03, only the "full", "angle", "atomic", "charge", "sphere", "dipole", "ellipsoid", and "molecular" styles have been tested. Other non-point-like atoms like "tri", "line" *should* also work with moltemplate. However these objects are *not rotated correctly* by the ".rot()" command (or scaled correctly by the ".scale()" command). More exotic exotic atom styles, such as "wavepacket", "electron", "sphere" and "peri" have not been tested. In addition, atom_style **body** and atom_style **template** are *not* supported. Feel free to contact **jewett.aij@gmail.com** to request support for exotic atom styles.

4) When placed at the end of a line, LAMMPS interprets **the "&" character** as a request to merge two lines together. *It is usually safe to use this character inside moltemplate write() or write_once() commands.* However in some rare cases, joining two lines together using the "&" character can confuse moltemplate. For example, in a lammps input script command, (like "pair_coeff" or "dihedral_coeff"), **the "&" character should not appear before the last "@" or "$" variable is referenced.** Also avoid using the "&" character anywhere in the "Data Atoms", "Data Bonds", "Data Angles", "Data Dihedrals", "Data Impropers", "Data Angles By Type", "Data Dihedrals By Type", and "Data Impropers By Type" sections.

5) Triclinic boundary conditions have not been tested:

As of 2019-9-03, support for PDB files with triclinic cells is experimental. Please let me know if it is not working.

6) Inconsistent support for wildcard characters ("*" and "?") The wildcard character "*" is interpreted differently in different parts of an LT file. Wildcard characters work reliably and are used for *string* pattern matching when inside "bond_coeff", "angle_coeff", "dihedral_coeff", "improper_coeff",

and most "pair_coeff" commands, as well as any of the *"By Type"* sections in an LT file (such as *"Data Angles By Type"*, *"Data Dihedrals By Type"*, and *"Data Impropers By Type"*). However these wildcard characters *do not* within pair_coeff commands that require *more* than 2 atom types as arguments. (such as "pair_style hbond/dreiding/lj". However manybody pair_styles which use "pair_coeff * *" notation work fine.)

Appendices

A Bonded interactions "By Type"

Interactions between atoms in LAMMPS which are not bonded together (ie "non-bonded" or "pair" interactions) are specified *by atom type. Bonded interactions* in LAMMPS, (including 3-body angle, and 4-body dihedral and improper interactions), are specified by unique *atom ID number.* (There are typically a large number of angles and bonds in a typical molecule, and this information occupies the majority of in a typical LAMMPS data file.)

This has changed in moltemplate.sh. moltemplate.sh contains a utility which can generate angles, dihedrals, and impropers automatically by atom and bond *type.* (This utility is described in section F.) moltemplate.sh will inspect the network of bonds present in your system, detect all 3-body, and 4-body interactions, and determine their type. (Higher n-body interactions can also be defined by the user.) Specifying interactions this way can eliminate significant redundancy since many atoms share the same type.

To make use of this feature, you would create a new section named "Data Angles By Type", "Data Dihedrals By Type", or "Data Impropers By Type" whose syntax mimics the "Angles", "Dihedrals", and "Impropers" sections of a LAMMPS data file. The syntax is best explained by example:

```
write("Data Angles By Type") {
  @angle:XCXgeneral       *      *C*      *
  @angle:CCCgeneral    @atom:C @atom:C @atom:C    *          *
  @angle:CCCsaturated  @atom:C @atom:C @atom:C @bond:SAT @bond:SAT
}
```

The first line will generate a 3-body angle interaction (of type "@angle:XCXgeneral") between any 3 consecutively bonded atoms as long as the second atom's type-name contains the letter "C". (Atom and bond type-names can contain wildcard characters *)

The second line will generate a 3-body interaction of type "@angle:CCCgeneral" between any 3 atoms of type "@atom:C", regardless of the type of bonds connecting them. (The last two columns, which are both wildcard characters, *, tell moltemplate.sh to ignore the two bond types. Since this is the default behavior these two columns are optional and can be omitted.)

The third line will generate a 3-body interaction of type "@angle:CCCsaturated" between any 3 atoms of type "@atom:C", if they are connected by bonds of type "@bond:SAT".

Note: The 2nd and 3rd lines in this example will generate new interactions which may override any angle interactions assigned earlier.

A.1 Regular expressions

Regular-expressions can also be used to match potential atom and bond types. To use regular expressions, the first 3 characters following ":" should be "re.", and the variable name should be enclosed in curly brackets, {}. For example: @{atom:re.C[1-5]}, should match @atom:C1 through @atom:C6.

*(**Note:** Moltemplate cannot understand regular expressions unless the number of '{ ' and '}' characters within them is **balanced**. (or if you preceed them with a backslash character). Moltemplate also cannot understand regular expressions containing whitespace. If you break these rules, moltemplate will get so confused that it will probably provide you with a confusing or misleading error message.)*

In a similar way, one can use regular expressions in "Dihedrals By Type" and "Impropers By Type".

Note: This is an experimental feature. Regular expressions have not been tested as of 2020-11-04.

B Using ltemplify.py to create an *LT file*

The "ltemplify.py" script is used to convert LAMMPS data files and input scripts into a single MOLTEMPLATE ("**LT**") file.

Typically, the LT files generated by "ltemplify.py" contain the definition of a single type of molecule (or molecular complex) present in the data file. This way, moltemplate users later on can build complicated simulations using this molecule as a building block (perhaps along with other molecules).

Users can select the molecule (or molecules) they want using the "-mol", "-id", or "-type" arguments, and give the molecule a name using the "-name" argument. (See below.) The resulting LT file will include all of the information relevant to that molecule including atom types, charges, coordinates, bonded interactions, force field parameters, force field styles, groups, and fixes that effect the molecule. (Other information will be omitted.)

However, by default, "ltemplify.py" will copy all of the information from these files into an LT file that describes the entire system. *(Later, when moltemplate.sh is run on that LT file, it will try to re-generate all of the original LAMMPS files.)* Normally, this is not very useful.

Typical Usage

```
ltemplify.py -name MoleculeName -mol MolID INPUT_SCRIPT DATA_FILE > FILE.lt
```

...where *MoleculeName* is a string, *MolID* is an integer, *INPUT_SCRIPT* and *DATA_FILE* are the names of a LAMMPS input script and a data file containing the molecule of interest, and *FILE.lt* is the resulting MOLTEMPLATE file created by ltemplify.py. (See section B.1 for more information.)

Note: Tiresome details to follow.

First time readers should probably skip to the examples in sectionB.4.

Required arguments

"ltemplify.py" requires only one argument: the name of a LAMMPS data file. However (as shown in the example above), it also reads LAMMPS input scripts. *(Note: If LAMMPS input scripts are included, they must*

*appear **before** the DATA file in the argument list. See examples below.)* "ltemplify.py" also accepts many arguments to select the atoms belonging to the molecule of interest and customize the output.

LAMMPS input scripts

In addition to LAMMPS DATA files, users can also supply one or more LAMMPS input scripts (typically containing information relevant to that molecule, such as force field parameters and fixes). If LAMMPS input scripts are included, they must appear *before* the DATA file in the argument list. (See examples below.)

B.1 Optional arguments

argument	meaning
-name *NAME*	Specify the name of the molecule described in the output file. (The optional "inherits" keyword can be used to select a force field.)
-atomstyle *style*	Optional: Force ltemplify.py to use a particular atom_style. (Hybrid styles should be surrounded by quotes, eg *-atomstyle "hybrid full dipole"*.)
-columns *"column_list"*	For custom atom_styles, you can list of column names in the "Atoms" section manually. (For example: **-columns "molid x y z atomid atomtype mux muy muz"**)
-mol *"molID_list"*	Select the molecule you want to appear in in the resulting LT file. To select more than one molecule, supply a list of numbers surrounded by quotes.
-id *"id_list"*	Select atoms by their atom-IDs. Use quotes to surround the list of atom ID numbers. Unselected atoms will be omitted.
-type *"type_list"*	Select atoms by their types. Use quotes to surround the list of atom type numbers.
-datacoeffs	Put force field information in the data file, not in an input script. (By default, force field parameters will be placed in the "In Settings" section which will eventually be written to a LAMMPS input script.)
-ignore-comments	Do not infer atom, bond, angle, dihedral, and improper type names from comments in the data file.
-ignore-coeffs	Ignore all force field parameters (coeffs).
-ignore-angles	Ignore angles, dihedrals and impropers. Omit from output file. (This is useful when using external force fields, such as OPLSAA.)—
-ignore-bond-types	Ignore the 2nd column in the "Bonds" section of the LAMMPS data file, and create a "Bond List" section in the resulting MOLTEMPLATE LT file which omits the bond types. (This is useful when using external force fields, such as OPLSAA.)—
-ignore-masses	Ignore all masses in the data file. Omit from output file. (This is useful when using external force fields, such as OPLSAA.)—
-prepend-atom-type *STR*	prepend the string from the *STR* argument to the beginning of all atom type names.

Examples showing argument usage are included in section B.4.

Default behavior

*Note that by default (if the "-mol", "-id", or "-type" arguments are omitted), "ltemplify.py" will copy **all** of the information from the LAMMPS files into an LT file that describes the entire system. Normally, this is not very useful.*

Details

All atoms, bonds, angles, dihedrals, and impropers and their associated types will be converted to moltemplate "$" or "@" counter variables (and the relevant portion of each file will be moved to sections with the correct header names). Coefficients, atom styles, and most force-field styles and settings *should* also be included in the resulting .LT file. ltemplify.py also understands simple group commands (using "id", "molecule", or "type" styles) and "fix shake", "fix rattle" and "fix rigid" (untested 2019-9-03). However most other fixes, and complex group commands are not understood. Those commands must be added to the resulting .LT file manually. (See section B.5 for more details.)

B.2   Fixes and Groups

ltemplify.py has *limited* support for "fix" and "group" commands, including "fix shake", "fix rattle", "fix rigid", and "fix poems". Other fixes must be added manually to the file generated by ltemplify.py. (Such as fix "restrain", "bond/create", "bond/break", "bond/react", "ttm", etc...)

ltemplify.py can understand simple (static) "group" commands, and will include them in the output file, if it can determine that they contain any relevant atoms. (Fixes depending on irrelevant groups are also deleted.)

Note: This feature has not been tested carefully. So please review all of the group and fix commands generated by ltemplify.py to make sure they refer to the correct atoms. And please report any bugs you find. (-Andrew 2019-9-03)

Automatic generation of atom, bond, angle, dihedral, improper names

By default ltemplify.py generates atom, bond, angle, dihedral, and improper, type names and id names automatically. This resultis in atoms with types like "@atom:type3", and IDs like "$atom:type3_7" (I.e. the 7th atom of type 3.)

Inferring atom type names from comments

However, ltemplify.py uses comments in the "Masses" section of the LAMMPS DATA file (if present) to determine the name of each atom type. Consider the following excerpt from a hypothetical data file:

```
Masses
```

```
1 12.01  # c3
```

```
2 1.008  # h3
3 1.008  # ho
4 16.00  # oh
```

This means atoms of types 1, 2, 3, and 4 will be referred to as "@atom:c3", "@atom:h3", "@atom:ho" and "@atom:oh", respectively in the moltemplate (LT) file created by ltemplify.py.

Ignoring comments

The "*-ignore-comments*" argument will disable this behavior and assign numeric names to the atom types in the usual way (eg "*@atom:type1*", "*@atom:type2*", "*@atom:type3*", "*@atom:type4*").

Bond, Angle, Dihedral, and Improper type names

Similarly, by default, bonds and angles are automatically assigned to type names like "@bond:type4", "@angle:type7".

However, if comments appear directly following the line in the header file "*N* bond types", then these comments will be interpreted as a list of bond type names (optionally preceded by an integer). (The same is true of angle, dihedral, and improper type names.) Consider this excerpt from a LAMMPS data file:

```
2 atom types
# c3
# h3

2 bond types
# CCethane
# c3_h3

2 angle types
# c3_c3_h3
# h3_c3_h3
```

In this example, bonds of type 1 and 2 will be referred to as "@bond:CCethane" and "@bond:c3_h3" in the moltemplate file, respectively. Similarly, angles of type 1 and 2 will be referred to as "@angle:c3_c3_h3" and "@angle:h3_c3_h3", respectively. (As in the previos example, atoms of type 1 and 2 will be referred to as "@atom:c3" and "@atom:h3" respectively. You can specify atom type strings *either* here, or in the Masses section.)

(As before, the "*-ignore-comments*" argument will disable this behavior.)

If you forget to add comments to the LAMMPS data file before running *ltemplify.py*, you can always use a text-editor (or *sed*) to manually find and replace all instances of "@atom:type1" with something more meaningful, like "@atom:c3", for example.

B.3   Force fields

Some data files contain a list of *angle, dihedral, or improper* bonded interactions. If so, then by default *ltemplify.py* will include this information in the moltemplate (LT) file that it creates. Sometimes, data files lack this information.

Either way, force fields (including "OPLSAA", "GAFF2", and "COMPASS"), contain rules for generating these interactions automatically. Hence, users may intentionally wish to exclude this information from the moltemplate files that ltemplify.py generates when this information is contained in the force field they want to use. (They can do this using the "-ignore-coeffs", "-ignore-angles", and "-ignore-bond-types" arguments explained below.)

Using the inherits keyword to specify force fields

Moltemplate provides several different force fields to choose from (such as OPLSAA, GAFF2, or COMPASS). In addition, users can create their own custom force-fields. To use these force fields, you must specify the one you want to use using the *-name* argument with the *inherits* keyword ("**-name** "MOLECULE_NAME inherits FORCE_FIELD"") For example:

```
ltemplify.py -name "Ethane inherits GAFF2" \
             -ignore-coeffs \
             ethane.data > ethane.lt
```

This will ask ltemplify.py to create a file defining molecule named "Ethane". Later when moltemplate is used to read this file, the "GAFF2" force field will be used to generate angles, dihedrals and impropers, and lookup their force field parameters.

In addition, after ltemplify.py is finished, the user must manually insert the following line *at the beginning* of the file that ltemplify.py created. For example:

```
import "gaff2.lt"     #<-- define the GAFF2 force field


# --- the text below was generated by ltemplify.py ---
Ethane inherits GAFF2 {
  ...
}
```

ltemplify.py does not do this for you. A list of available force fields can be found in the "moltemplate/force_fields/" directory distributed with moltemplate on github.

-ignore-coeffs

The optional "*-ignore-coeffs*" argument will force ltemplify.py to ignore the force field parameters that it encountered in the user's input script or DATA file. The resulting LT file will omit this information. If you plan to use a force field with this molecule, then this information will be present in the force field you are using, so there's no need to include it in the resulting LT

file you are creating now. (Later when you run moltemplate.sh on the LT file that ltemplify.py created, it will use the force field to lookup these force field parameters.)

-ignore-angles

If the original DATA file has "Angles", "Dihedrals", or "Impropers", you can use the "*-ignore-angles*" argument if you want to force ltemplify.py to ignore/remove those interactions from the LT file which ltemplify creates. (Doing that will allow the force field rules to take precedence later when we run moltemplate.sh on that file.)

-ignore-bond-types

Similarly, when using force-fields, you only need to specify a list of *which pairs of atoms* are bonded together. The force-field will determine the type and properties of each bond (eg, equilibrium rest length, stiffness, etc...) according to atom type names and the force field rules.

To do that, you must force *ltemplify.py* to ignore the existing bond type information present in your data file using the "*-ignore-bond-types*" argument. This will force ltemplify.py to ignore the bond types in the (2nd column of the) "Bonds" section of the LAMMPS data file that you provided. In this way, the bond type can be determined later by moltemplate.sh in a way which is consistent with the force field you selected.

See section B.4 for examples.

Disclaimer

ltemplify.py is experimental software. The lemplify.py script has limited understanding of all of the features available in LAMMPS. Please look over the resulting ".LT" file and check for errors. (If necessary, convert any remaining atom, bond, angle, dihedral, or improper id or type numbers to the corresponding $ or @ variables.) Some exotic pair styles which have their own special syntax are not understood. These coeffs must be converted manually. Support for "group" and "fix" commands is also limited. (See section B.2.) Please report errors in the behavior of ltemplify.py.

B.4   Examples

Example 1

```
ltemplify.py -name Ethane -molid "1" FILE.in FILE.data > ethane.lt
```

This example creates a new file ("ethane.lt") containing a new type of molecule (named "Ethane"), consisting of all the atoms whose molecule-ID number equals 1. *(Presumabely, the first molecule in FILE.data is an ethane molecule.)*

ltemplify.py reads the atom coordinates and bonded interactions from "FILE.data". Other information relevant to that molecule (including the

atom_style, force-field styles and parameters, groups and fixes) are read from "FILE.in" (which is presumably a LAMMPS input script file).

(NOTE: Again, it is not necessary to include a LAMMPS input script in the argument list. However important information is typically contained in LAMMPS input script files, so if you have one, including it is recommended. However a data file is enough.)

Note: Selecting atoms by molecule-ID only works if you are using one of the "molecular" atom_styles (such as "atom_style full"). If you are using a different atom_style (such as "atom_style angle" or "atom_style bond"), you can select the atoms you want either by type or by id number. (See below.)

Example 2

Sometimes, the information describing your molecule will divided into multiple lammps input scripts. (For example, one input script may contain various *style* commands. The next input script may contain *coeff* commands.) In that case, these input scripts should appear in the argument list *before the data file*, and in the order in which they are read by LAMMPS.

```
ltemplify.py -name Ethane \
             -molid "1" \
             FILE1.in FILE2.in FILE.data > ethane.lt
```

Example 3

```
ltemplify.py -name Ethane -molid "1" \
             -id "13 14 15 61*69" \
             FILE.in FILE.data > ethane.lt
```

In this example, only atoms whose ids are 13, 14, 15, and 61 through 69 are included.

Example 4

```
ltemplify.py -name Ethane \
             -atomtype "1 2 3" \
             FILE.in FILE.data > ethane.lt
```

In this example, only atoms whose type is 1, 2, or 3 are included.

Example 5

```
ltemplify.py -name EntireSystem FILE.in FILE.data > entire_system.lt
```

This creates a template for a new molecule object (named "EntireSystem"), consisting of **all** the atoms in the lammps files you included, and saves this data in a single LT file ("entire_system.lt"). This file can be used with moltemplate.sh (and/or ttree.py) to define large systems containing this molecule.

Note: Again, the input scripts ("FILE.in" in this example) should appear before the data file ("FILE.data") in the argument list.

You can also use *ltemplify.py* to create molecules that use 3rd-party force fields such as OPLSAA, GAFF2, COMPASS, ...

Example 6

This example demonstrates how to build a molecule using the "GAFF2" force field. The following example extracts molecule 1 from "FILE.in" and "FILE.data".

```
# This example creates a new file, "ethane.lt", which will contain the
# instructions for building a "Ethane" molecule using "GAFF2". First
# specify which file contains the definition of the "GAFF2" force field:

echo "import gaff2.lt"  >  ethane.lt


# Then use ltemplify.py to extract information from FILE.in, FILE.data

ltemplify.py -name "Ethane inherits GAFF2" \
             -molid "1" \
             -ignore-angles -ignore-bond-types -ignore-coeffs \
             FILE.in FILE.data >> ethane.lt


# Note: if you want to build a simulation containing these molecules,
# you will have to create a "system.lt" file which refers to "ethane.lt"
# and then run moltemplate.sh on this file.
```

As mentioned earlier, comments in "file.data" will determine the name of each atom type and *should match atom type names in the force field*.

In this example, the angle, dihedral, improper, and bond-type information is stripped from the original file.data (and will be generated later according the the rules defined in the "GAFF'2' force field). The name of the molecule ("Ethane inherits GAFF2") includes a reference to the force field ("GAFF2") which will be used to lookup this information. (Note: The "GAFF2" force field parameters are typically defined in a file named "gaff2.lt". Hence in this example we used "echo" to insert a link to "gaff2.lt" at the beginning of the "ethane.lt" file so that moltemplate.sh will know where to find them. Alternatively, this could be done manually by the user.)

B.5   Known bugs and limitations (ltemplify.py)

Exotic styles are not supported

ltemplify.py does **not** understand the syntax of exotic many-body pair_styles such as tersoff, sw, meam, reax, dpd, edip, dipole, lubricate, hbond/dreiding (even though these styles are supported by moltemplate). After running ltemplify.py, the user must manually edit the resulting ".lt" files. For example: ltemplify.py will not understand wildcard characters ("*" characters) which typically appear in the "pair_coeff" commands or "Pair Coeffs" section when using these many-body pair styles. You will have to remove the

extra lines automatically generated by ltemplify.py and put the wildcard characters back (eg "pair_coeff * * ...") manually. (Later the user may need to run moltemplate using the appropriate "-a" command line args to make sure the various atom types are assigned to the correct numbers. This is usually needed in order to keep them consistent with the order of parameters in the corresponding pair style's input files. See section D.1.) In addition, auxiliary atom types (such as the "hydrogen" atom type required by hbond/dreiding) will not even be parsed. If you are using the "hbond/dreiding" pair style, you will have to manually specify the atom type for the hydrogen-atom mediator in every "pair_coeff" command after running ltemplify.py

Wildcard characters ("*") expansion

As explained in section 11, moltemplate is often confused whenever wildcard characters ("*" characters) appear inside any of the the "coeff" commands (or "Coeff" sections of the data file). So ltemplify.py attempts to remove these characters and expand these commands, generating multiple lines of output, and listing each atom type explicitly. (This is also done for bond types, angle types, dihedral types, and improper types.) This may not be what you want. (For example, this can be a problem if you are using a many-body pair style which requires you to specify "* *" for the atom types, such as *tersoff*, *eam*, or *sw*.)

C Visualization in VMD

This appendix is only intended to give you a quick, minimal list of features you need to know to display your molecules using VMD. These instructions were written for VMD 1.9 and topotools 1.2. For advanced VMD features, analysis, and rendering options, consult the official VMD documentation at `http://www.ks.uiuc.edu/Research/vmd/current/docs.html`

C.1 Customizing the appearance in VMD

By default, VMD is likely to display your molecules with points and lines, which can be ugly and difficult to see. To alter the appearance of your molecules, select the **Graphics→Representations...** menu, and then select an option from the **Drawing Method** pull-down menu. Atoms are colored by atom-type by default. You can customize the color of each atom type by **Graphics→Colors...** As of 2019-9-03, VMD arbitrarily allows you to assign colors to *only* the first 9 atom types. However you can get around this limitation using multiple *representations* customize the appearance of the remaining atom types (as explained below).

You may wish to use different representations for different molecules or atom types. To do this, select the **Graphics→Representations...** menu and click on then **Selections** tab. Then click on the **Create Rep** button to create multiple "*representations*" of your system. For each *representation*, you can select different sets atoms, and use different draw-styles, for those

atoms. For example, you can customize the color of these atoms manually by choosing **ColorID** from the **Coloring Method** pull-down menu. Then, to the right of this menu, you can select the color (which is represented by a number). This will effect all of atoms in the current *representation*. You can also select a different **Draw Style** and alter the atom and bond radii.

You can select from the the list of *representations* you have already created by clicking on the list under the **Create Rep** button. (Double-clicking temporarily hides a *representation* from view.)

Again, each *representation* is usually assigned to a different subset of atoms from the system. To specify the atoms in each *representation*, click on the **Selections** tab. By default "all" atoms are selected, however you can select atoms according to atom **type**, **index**, **molid**, **charge**, **mass**, **x**, **y**, **z**. This will limit the current display settings to a subset of the atoms/bonds present in your system. When selecting atoms, you can use complex boolean expressions (containing one or more *and* and *or* operators and parenthesis). For more information and some examples, see `http://www.ks.uiuc.edu/Research/vmd/vmd-1.9/ug/node19.html` and `http://www.ks.uiuc.edu/Research/vmd/vmd-1.9/ug/node87.html#ug:topic:selections`.

Note: In VMD/topotools, the **type**, **index**, and **molid** properties of each atom correspond to the *@atom*, *$atom*, and *$mol* variables for each atom in moltemplate. Unfortunately, VMD does not understand moltemplate variable naming syntax (discussed in section 5.2). Instead, in VMD, variables must be specified by their numeric equivalents. You can determine these numbers by reading the *output_ttree/ttree_assignments.txt* file. (See section D.1 for details.) That file contains a table containing a list of the numbers assigned to each *@atom* (type), *$atom* (id), and *$mol* (molecule-id) variable.

C.2   Visualizing periodic boundaries

To view the periodic box boundaries, select the **Extensions→Tk Console** menu, and in the *Tk Console* window, enter:

```
pbc box
```

Note that the molecules in your system might not lie inside this box. You can *wrap* them inside the box using this command:

```
pbc wrap -compound res -all
```

You may wish to center the box around a molecule. There are several ways to do this. You can move the box manually this way:

```
pbc wrap -compound res -all -shiftcenterrel {0.0 0.15 0.0}
pbc box -shiftcenterrel {0.0 0.15 0.0}
```

This will shift the position of the box by 15% in the Y direction. (Distances are measured in units of box-length fractions, not Angstroms.)

(Advanced usage: if you have a solute whose atoms are all of type "1", surrounded by a solvent of atoms of type "2" then you can also try this to center the box around it using: "pbc wrap -sel type=1 -all -centersel type=2

-center com". The "1" and "2" are the @atom type numbers assigned by moltemplate. This can be found in the output_ttree/ttree_assignments.txt file. If you are viewing a trajectory, then this will modify the appearance of every step in the trajectory, centering the box around the solute atoms.)

For more details visualizing periodic-boundaries, visit: `http://www.ks.uiuc.edu/Research/vmd/plugins/pbctools`

To prevent atom overlap, you should also check if your periodic boundary conditions are too small. To do that:

    a) select *Graphics→Representations* menu option

    b) click on the "Periodic" tab, and

    c) click on the **+x**, **-x**, **+y**, **-y**, **+z**, **-z**, and **self** checkboxes.

When doing so, inspect the system to make sure the atoms which appear occupy non-overlapping volumes in space.

D   Advanced moltemplate.sh Usage

moltemplate.sh has several optional command line arguments. These are explained in below:

```
Usage:

moltemplate.sh [-atomstyle style] \
               [-pdb/-xyz/-raw coord_file] \
               [-a assignments.txt] file.lt


Optional arguments:

-atomstyle style  By default, moltemplate.sh assumes you are using the "full"
                  atom style in LAMMPS.  You can change the atom style to "dipole"
                  using -atomstyle dipole.  If you are using a hybrid style,
                  you must enclose the list of styles in quotes.  For example:
                  -atomstyle "hybrid full dipole"
                  For custom atom styles, you can also specify the
                  list of column names manually (enclosed in quotes):
                  -atomstyle "molid x y z atomid atomtype mux muy muz"
                  Be careful to enclose the entire list in quotes(").

-raw raw_file   The raw_file file should contain the atomic coordinates in RAW format
                RAW files are simple 3-column ASCII files containin the coordinates
                for the atoms in the system. (One line per atom, 3 numbers per line.
                The atoms must appear in the same order in the data file.)
-xyz xyz_file   An xyz_file argument should be supplied as an argument
                following "-xyz".
                This file should contain the atomic coordinates in xyz format.
                (The atoms must appear in the same order in the data file.)
```

```
-pdb pdb_file    The pdb_file file should contain the atomic coordinates in PDB format

                 This file should contain one ATOM or HETATM record per atom.   Atoms

                 are sorted by chainID, resID, insertCode, atomID (in that order).
                 This order must match the order the atoms appear in the data file.

                 If the PDB file contains periodic boundary box information
                 (IE., a "CRYST1" record), this information is also copied
                 to the LAMMPS data file.
                 (Support for triclinic cells is experimental as of 2019-9-03.
                 Other molecular structure formats may be supported later.
-a "@atom:x 1"
-a assignments.txt
                 The user can customize the numbers assigned to atom, bond,
                 angle, dihedral, and improper types or id numbers by using
                     -a "VARIABLE_NAME VALUE"
                 for each variable you want to modify.  If there are many
                 variables you want to modify, you can save them in a file
                 (one variable per line).  For an example of the file format
                 run moltemplate.sh once and search for a file named
                 "ttree_assignments.txt".  (This file is often located in
                 the "output_ttree/" directory.) Once assigned, the remaining
                 variables in the same category will be automatically assigned
                 to values which do not overlap with your chosen values.
-b assignments.txt
                 "-b" is similar to "-a". However, in this case, no attempt
                 is made to assign exclusive (unique) values to each variable.
-nocheck
                 Normally moltemplate.sh checks for common errors and typos and
                 halts if it thinks it has found one.  This forces the variables
                 and categories as well as write(file) and write_once(file)
                 commands to obey standard naming conventions.  The "-nocheck"
                 argument bypasses these checks and eliminates these restrictions.
-checkff
                 This cause moltemplate.sh to check to make sure that there
                 are valid angle and dihedral interactions defined for every
                 3 or 4 consecutively bonded atoms in the system
                 (defined in "Angles/Dihedrals By Type").
```

D.1 Manual variables assignment ("-a" or "-b")

It is possible to manually customize the values assigned to the atom types (or
to any other ttree-style variables). For example, consider the the "spce.lt"
file shown earlier. This file defines a single water molecule with two atom
types (hydrogen and oxygen). Typically the "O" atom type is normally
assigned to the integer "1", and "H" would be assigned to "2". This is
because "O" appears before "H" in that file. If you wanted to swap the

order, you could swap the order in which they first appear.

Alternately you can specify the atom assignments directly using one or more "-a" flags followed by a quoted assignment string:

```
moltemplate.sh -a '@atom:SPCE/O 2' system.lt
```

This assigns the oxygen atom type to "2". Note that quotes are necessary around the '@atom:SPCE/O 2' string, which is a single argument. (Also note that it is necessary to include SPCE/ before the O, because in that example, this atom appeared (and was thus defined) inside the SPCE molecule's environment. Alternately, if it had been defined outside, globally, then you could refer to it using "@atom:O")

Variables need not be assigned to numbers. If for some reason, you want to substitute "a string" everywhere this atom type appears, you would do it this way:

```
moltemplate.sh -a '@atom:SPCE/O "a string"' system.lt
```

Multiple assignments can be made by using multiple "-a" flags:

```
moltemplate.sh -a '@atom:SPCE/O 2'  -a '@atom:SPCE/H 1' system.lt
```

However if you have a large number of assignments to make, it may be more convenient to store them in a file. You can create a two-column text file (for example "new_assignments.txt") and run moltemplate this way:

```
moltemplate.sh -a new_assignments.txt system.lt
```

The contents of the "new_assignments.txt" file in this example would be:

```
@atom:SPCE/O  2
@atom:SPCE/H  1
```

The order of lines in this file does not matter.

Assigning $angle, $dihedral, $improper variables

In general any kind of variable can be assigned this way (not only atom types), including $mol, $bond, @bond, @angle, $angle, ... as well as user-defined variable type. *Caveat: The only occasional exceptions are the $angle, $dihedral, $improper variables.* (When "Angles By Type" interactions are selected by the user, and mixed with regular "Angles", all of the $angle variables are automatically generated. The same is true for "Dihedrals By Type" and "Impropers By Type". See section F for an explanation of "By Type" interactions.)

Angles, dihedrals, and impropers interactions are automatically generated, and in this case the user does not have the freedom to assign these variables.

The "-b" flag

Note that when using the "-a" flag above, care will be taken to insure that the assignment(s) are exclusive. None of the atom types (other than @atom:SPCE/O) will be assigned "2". (For this reason, using the "-a" flag to change the atom type assignments can, in principle, alter the numbers assigned other atom types, or variables.) This usually the desired behavior. However suppose, for some reason, that you wanted to force a variable assignment, so that other variables in the same category are not effected. In that case, you can use the "-b" flag:

```
moltemplate.sh -b '@atom:SPCE/O 2' system.lt
```

Keep in mind, that in this example, this could cause other atom-types (for example "@atom:SPCE/H") to be assigned to overlapping numbers.

The "ttree_assignments.txt" file

Generally, after running moltemplate.sh, a "ttree_assignments.txt" file will be created (or updated if it is already present) to reflect any changes you made. (This file is usually located in the "output_ttree/" directory. It can also be located the current directory "./".) You can always check this to make sure that the atom types (or any other ttree variables) were assigned correctly.

The "ttree_assignments.txt" file has the same format as the "new_assignments.txt" file example above.

Note: In both files, an optional slash, "/", may follow the "@" or "$" characters, as in "@/atom:SPCE/O". (This slash is optional and indicates the environment in which the counter is defined. The "@atom" counter is defined globally. The "$resid" counter example described in section D.2 is not.)

Bug-warning: Using the "delete" command may cause some of the instance variables (specifically the $atom, $mol, $bond, $angle, $dihedral, and $improper variables) to be numbered incorrectly. However static variables (beginning with @) should always be accurate. -Andrew 2019-9-03.

lttree.py and ttree.py also accept "-a" and "-b" flags

If for some reason, you are using "lttree.py" or "ttree.py" instead of "moltemplate.sh", then the "-a" and "-b" flags explained here also work with these scripts. They are not specific to moltemplate.sh.

D.2 Customizing the counting method using *category*

Variables in ".lt" files are assigned to integers by default, starting with 1, and incrementing by 1. This can be overridden using the "category" command. For example, to create a new variable category named "distance" which starts at 0 and increments by 0.5, you would include this command in your LT file:

```
category $distance(0.0, 0.5)
```

(This command should *not* be used with traditional counter categories like *$atom, $bond, $angle, $dihedral, $improper, $mol, @atom, @bond, @angle, @dihedral,* and *@improper.*)

D.3   Creating local independent counters

By default variables in a given category are always assigned to unique integers. This can be overridden using the "category" command. For example, you might have a variable that keeps track of the monomer in every polymer. The first monomer in a polymer is assigned "1", the second monomer, "2", etc, *regardless* of the number of polymer in your system.

To do this, we can create a new variable category named "monomerid" which is defined within the scope of each instance of the "Polymer" molecule:

```
Monomer {
  write("Data Atoms") {
    $atom:ca @atom:CA $monomerid:.  0.0  0.0 0.0 0.0
    $atom:cb @atom:CB $monomerid:.  0.0  1.53 0.0 0.0
  }
}


Polymer {
  category $monomerid(1,1)
  monomers = Monomer[100]
}


polymers = Polymer[10]
```

In this example, there are 10 polymers containing 100 monomers each. The "$monomerid" counters will be replaced with integers in the range $1 \ldots 100$, (not $1 \ldots 1000$, as you might expect). Because the "$monomerid" counter is local to the protein it is defined within, "$monomerid" variables in other proteins do not share the same counter, and can overlap.

D.4   Counting order

Most variables are assigned automatically. By default static variables (@) are assigned in the order they appear in the file (or files, if multiple LT files are included). Subsequently, instance variables ($) are assigned in the order they are created during instantiation. However you can customize the order in which they are assigned.

Ordering

LT files are parsed by moltemplate.sh/lttree.py in multiple stages. The "write_once()" and "write()" commands are carried out in the static and instance phases respectively, as explained below.

The *static* phase

In the "static" phase, "write_once()" statements are carried out in the order they are read from the user's input file(s) (regardless of whether or not they appear in nested classes). Any "include" commands will effect this order. After processing the class definitions, and carrying out the "write_once()" commands, lttree.py begins the instantiation phase.

The *instantiation* phase

During this phase, lttree.py makes copies of (instantiates) classes which were requested by the user using the "new" command. During this stage, lttree.py also appends data to files using the "write" command. (In this manual, the "write()" and "new" are called instance commands.) The sequence of alternating "write()" and "new" commands in the order that they appear in the user's input file(s). "new" commands recursively invoke any instance commands for each copy of the class they create.

Again, the counting of instance variables (prefixed by "$") does not interfere with static variable assignment. For example "@atom:x" and "$atom:x" correspond to different variables and belong to different variable categories ("@atom" and "$atom") and they are assigned to numerical values independently.

E   Using *lttree.py* or *ttree.py* directly

(bypassing moltemplate.sh)

"moltemplate.sh" is only a simple script which invokes "lttree.py", and then combines the various output files generated by lttree.py into a single LAMMPS input script and a data file, along with coordinate data. "lttree.py" then invokes "ttree.py". "ttree.py" lacks the ability to read or generate coordinates, but is otherwise nearly identical to "lttree.py" and "moltemplate.sh".

If in the future moltemplate.sh no longer works with some new, recently added LAMMPS feature, you can bypass moltemplate.sh and run lttree.py or ttree.py directly. Everything moltemplate.sh does can essentially be done by hand with a unix shell and a text editor. This procedure is outlined below.

E.1   First run ttree.py

The syntax for running "ttree.py" is identical to the syntax for running moltemplate.sh. The moltemplate.sh syntax is explained above.

Unfortunately, ttree.py does not understand the -pdb, -xyz, or -raw arguments for processing coordinate data. If you run "ttree.py" directly, then you must extract the coordinate data from these files yourself and insert it into your lammps input files manually. This is explained below.

Example: Go to the examples/waterSPCE/ directory and run:
ttree.py system.lt

This will prepare LAMMPS input files for a system of 32 water molecules. (In this example, we are using the "SPCE" water model.)

Running the command above will probably create the following files: "Data Atoms" (The "Atoms" section of a LAMMPS data file, w/o coordinates) "Data Bonds" (The "Bonds" section of a LAMMPS data file) "Data Angles" (The "Angles" section of a LAMMPS data file) "Data Masses" (The "Masses" section of a LAMMPS data file) "In Init" (The "Initialization" section of a LAMMPS input script.) "In Settings" (The "Settings" section of a LAMMPS input script, which typically contains force-field parameters, group defs, and constraints) "Data Boundary" (The "Periodic Boundary Conditions" section of a LAMMPS data file.) "ttree_assignments.txt" (Variable assignments. See "customization" section.)

This data can be easily combined into a single LAMMPS data file and a single lammps input script later on, using a text editor, or the unix "cat" and "paste" commands.

It may also create these files: "Data Angles By Type", "Data Dihedrals By Type", "Data Impropers By Type". These files tell moltemplate how to automatically generate bonded-interactions by atom and bond type. They must be converted to lists of angles, dihedrals, and impropers, using the "nbody_by_type.py" utility (as explained in appendix A).

E.2   Then create a LAMMPS data file

Create a new file ("system.data" in this example), and paste the following text into it:

Create the "header" section

Example:

```
LAMMPS Description

    96  atoms
    64  bonds
    32  angles
    0  dihedrals

    2  atom types
    1  bond types
    1  angle types
    0  dihedral types


  0.000000    9.043     xlo xhi
  0.000000    15.663    ylo yhi
  0.000000    7.361     zlo zhi
```

If you use ttree.py, will have to count the number of atoms, bonds, and atom types, bond types etc. yourself.

Note: the numbers in the "xlo xhi" "ylo yhi" "zlo zhi" lines determine the simulation box size, and will vary from system to system. If ttree created

a file named "Data Boundary", you can copy this information from there. (Triclinic cells have a fourth line containing the "xy xz yz" parameters.) (If you have a .PDB file, these boundary box numbers are in the "CRYST1" line near the beginning of the file.)

Once you've created the "header" section of the data file, paste the other sections to the end of your LAMMPS data file (with the appropriate section headings and blank lines).

```
echo "" >> system.data
echo "Atoms" >> system.data
echo "" >> system.data
cat "Data Atoms" >> system.data
echo "" >> system.data
echo "Bonds" >> system.data
echo "" >> system.data
cat "Data Bonds" >> system.data
echo "" >> system.data
echo "Angles" >> system.data
echo "" >> system.data
cat "Data Angles" >> system.data
echo "" >> system.data
echo "Masses" >> system.data
echo "" >> system.data
cat "Data Masses" >> system.data
echo "" >> system.data
```

Depending on your system, you may also have these files as well: "Data Dihedrals" "Data Impropers" "Data Bond Coeffs" "Data Angle Coeffs" "Data Dihedral Coeffs" "Data Improper Coeffs". If so, then then append them to the end of your data file as well. (There are numerous other optional sections for "class2" force-fields. Exotic atom styles also require their own sections such as "lines" "ellipsoids" and "triangles". Consult the LAMMPS documentation for details on these as well.)

E.3 Now create the LAMMPS input script

```
echo "include \"In Init\"" > system.in
echo "read_data system.data" >> system.in
echo "include \"In Settings\"" >> system.in
```

Lastly, you have to worry about supplying the atomic coordinates. (Unlike moltemplate, ttree.py does not handle atom coordinates.)

The following commands are useful for extracting coordinates from PDB or XYZ files and converting them to LAMMPS input script commands:

E.4 Extract coordinates

To extract coordinates from a .PDB file ("file.pdb"), use:

```
awk '/^ATOM  |^HETATM/{print substr($0,31,8) \
                        " "substr($0,39,8) \
                        " "substr($0,47,8)}' \
    < file.pdb \
    > tmp_atom_coords.dat
```

(Note: There should be two spaces following the word "ATOM" above.)
    To extract coordinates from an XYZ file ("file.xyz"), use:

```
awk 'function isnum(x){return(x==x+0)} \
    BEGIN{targetframe=1;framecount=0} \
    {if (isnum($0)) {framecount++} else \
     {if (framecount==targetframe) { \
       if (NF>0) { \
        if ((NF==3) && isnum($1)) { \
         print $1" "$2" "$3} \
         else if ((NF==4) && isnum($2)) { \
         print $2" "$3" "$4} }}}}' \
    < file.xyz \
    > tmp_atom_coords.dat
```

E.5   Convert the coordinate file to LAMMPS input script format

```
awk '{if (NF>=3) { \
    natom++; print "set atom "natom" x "$1" y "$2" z "$3" "}}' \
    < tmp_atom_coords.dat \
   >> system.in.coords
```

Finally import "system.in.coords" in your lammps input script using:

```
echo "include \"system.in.coords\"" >> system.in
```

F   Using the *nbody_by_type.py* utility

(bypassing moltemplate.sh)

moltemplate.sh uses the "nbody_by_type.py" utility to generate many-body interactions between bonded atoms by atom type. In the event that moltemplate.sh crashes or is not up-to-date with LAMMPS, you can assign interactions by type by manually invoking nbody_by_type.py yourself.
    As an example, the following command will generate a file "Angles" containing lines of text which should eventually be pasted into the "Angles" section of a LAMMPS data file:

```
nbody_by_type Angles \
    -atoms "Data Atoms" \
    -bonds "Data Bonds" \
    -subgraph "nbody_Angles.py" \
    -nbodybytype "Data Angles By Type" \
    > "Data Angles"
```

For dihedral or improper interactions, repeat the command above, and replace "Angles" with "Dihedrals", or "Impropers" everywhere.

Note: The above instructions work assuming that you do not use any wildcard characters ("*" or "?") or regular expressions in your "Angles By Type" section. If you use wildcards or regular expressions, then you must run the program this way:

```
nbody_by_type Angles \
    -atoms "Data Atoms.template" \
    -bonds "Data Bonds.template" \
    -subgraph "nbody_Angles.py" \
    -nbodybytype "Data Angles By Type.template" \
    > "Data Angles.template"
```

Afterwards, you must then replace each variable in the "Angles.template" file with the appropriate integer before you copy the contents into the LAMMPS data file. (The ttree_render.py program may be useful for this. Open the moltemplate.sh file with a text editor to see how this was done.)

Note that "Data Atoms", and "Data Bonds" refer to files which are normally created by "ttree.py" or "lttree.py" which contain atom and bond data in LAMMPS data file format, respectively. Similarly "Data Angles By Type" refers to a file containing instructions for how to automatically generate angles by atom type. (Again, this would typically be generated by running "ttree.py" or "lttree.py" on an LT file containing a block of text wrapped inside a "write_once('Data Angles By Type')" command.)

Note: if you already have existing "Data Angles", you can add them to the list of angle interactions created by nbody_by_type.py.

```
nbody_by_type Angles \
    -atoms "Data Atoms" \
    -bonds "Data Bonds" \
    -subgraph "nbody_Angles.py" \
    -nbodyfile "Data Angles" \
    -nbodybytype "Data Angles By Type" \
    > extra_Angles.tmp
cat extra_Angles.tmp "Data Angles" > new_Angles
mv -f new_Angles "Data Angles"
rm -f extra_Angles.tmp
```

F.1 Usage

For reference, the complete man page for the "nbody_by_type.py" command is included below.

```
nbody_by_type.py reads a LAMMPS data file (or an excerpt of a LAMMPS)
data file containing bonded many-body interactions by atom type
(and bond type), and generates a list of additional interactions
in LAMMPS format consistent with those type (to the standard out).

Typical Usage:
```

```
nbody_by_type.py X < old.data > new.data

--or--

nbody_by_type.py X \
                -atoms atoms.data \
                -bonds bonds.data \
                -subgraph "nbody_X.py" \
                -nbody X.data \
                -nbodybytype X_by_type.data
                > new_X.data
```

In both cases "X" denotes the interaction type, which
is either "Angles", "Dihedrals", or "Impropers".
Support for other interaction types can be added by the user. See below.

Note: The optional "-subgraph" argument allows you to customize the
      rules used to match and generate interactions of that type.
      It is optional, and is only useful for forcefields which
      use non-standard dihedral or improper atom-order convetions.)

-------- Example 1 -------

```
nbody_by_type.py X < old.data > new.data
```

In this example, nbody_by_type.py reads a LAMMPS data file
"orig.data", and extracts the relevant section ("Angles",
"Dihedrals", or "Impropers"). It also looks a section named "X By Type",
   (eg. "Angles By type", "Impropers By type", "Impropers By type")
which contains a list of criteria for automatically defining additional
interactions of that type. For example, this file might contain:

Angle By Type

```
7 1 2 1 * *
8 2 2 * * *
9 3 4 3 * *
```

The first column is an interaction type ID.
The next 3 columns are atom type identifiers.
The final 2 columns are bond type identifiers.
The * is a wildcard symbol indicating there is no preference for bond types
in this example. (Optionally, regular expressions can also be used to
define a type match, by enclosing the atom or bond type in / slashes.)

    The first line tells us to that there should be a 3-body "Angle"
interaction of type "7" whenever an atom of type 1 is bonded to an atom

of type "2", which is bonded to another atom of type "1" again.
The second line tells us that an angle is defined whenever three atoms
are bonded together and the first two are of type "2".
(Redundant angle interactions are filtered.)

    New interactions are created for every group of bonded
atoms which match these criteria if they are bonded together
in the relevant way for that interaction type (as determined by
nbody_X.py), and printed to the standard output. For example,
suppose you are automatically generating 3-body "Angle" interactions using:

nbody_by_type Angles < old.data > new.data

The file "new.data" will be identical to "old.data", however the
"Angles By Type" section will be deleted, and the following lines of
text will be added to the "Angles" section:

394 7 5983 5894 5895
395 7 5984 5895 5896
396 7 5985 5896 5897
 : : :   :   :
847 9 14827 14848 14849

The numbers in the first column are counters which assign a ID to
every interaction of that type, and start where the original "Angles"
data left off (New angle ID numbers do not overlap with old ID numbers).
The text in the second column ("7", "9", ...) matches the text from the
first column of the "Angle By Type" section of the input file.

-------- Example 2 -------

nbody_by_type.py X \
                -atoms atoms.data \
                -bonds bonds.data \
                -subgraph "nbody_X.py" \
                -nbody X.data \
                -nbodybytype X_by_type.data \
                > new_X.data

In particular, for Angle interactions:

nbody_by_type.py Angles \
                -atoms atoms.data \
                -bonds bonds.data \
                -subgraph "nbody_Angles.py" \
                -nbody angles.data \
                -nbodybytype angles_by_type.data \
                > new_Angles.data

```
    When run this way, nbody_by_type.py behaves exactly the same way
    as in Example 1, however only the lines of text corresponding to
    the new generated interactions are printed, (not the entire data file).
    Also note, that when run this way, nbody_by_type.py does not read the
    LAMMPS data from the standard input.  Instead, it reads each section of
    the data file from a different file indicated by the arguments following
    the "-atoms", "-bonds", "-nbody", and "-nbodybytype" flags.

    "Angles" is a 3-body interaction style.  So when run this way,
    nbody_by_type.py will create a 5 (=3+2) column file (new_Angles.data).

Note: the atom, bond and other IDs/types in need not be integers.

Note: This program must be distributed with several python modules, including:
        nbody_Angles.py, nbody_Dihedrals.py, and nbody_Impropers.py.  These
     contain bond definitions for angular, dihedral, and improper interactions.
```

F.2   Custom bond topologies

Currently nbody_by_type.py can detect and generate "Angle" and "Dihe-dral" interactions between 3 and 4 consecutively bonded atoms. It can also generate "Improper" interactions between 4 atoms bonded with a T-shaped topology (one central atom with 3 branches). The nbody_by_type.py script imports external modules named "nbody_Angles.py", "nbody_Dihedrals.py", and "nbody_Impropers.py" to help it detect angles, dihedrals, and improper interactions automatically. In case any new interaction types are ever added to LAMMPS, it is easy to define new bonded interaction types by supply-ing a new "nbody_X.py" python modules. These python files are usually only a few lines long. Copy one of the existing modules "nbody_Angles.py", "nbody_Dihedrals.py", or "nbody_Impropers.py") and modify it to the sub-graph inside to match the bonded network that you want to search for.

G   Moltemplate Grammar

Moltemplate.sh is a script which invokes a python program program (*ttree.py*) to parse and interpret the moltemplate language. An overview of the gram-mar of that language is provided below. The grammer shown here is not comprehensive. The syntax of some lesser-used language features (such as varialble shortcuts, and paths containing "../" and "...") is omitted here (but discussed later in appendix G.1).

Note that the current language parser (*ttree.py*) was written by hand. (It was not generated by a compiler-compiler.) So it is unfortunately possible that some valid inputs may exist which satisfy the rules of the grammar and yet cause moltemplate to return an error message. However most moltem-plate commands are short and simple. Several years of heavy usage have passed since I have received a report of this kind of error.

Explanation of Terminals:

Terminals are the indivisible words and symbols in a language. Terminals in the moltemplate language fall into several categories.

```
Terminals ::= Integer | Number | String
```

- **Integer**: A nonnegative integer

- **Number**: A floating point number

- **String**: A string. (A sequence of characters.)

Strings fall into several categories:

```
String ::= InstanceName | ObjectTypeName | FileName | CategoryName | OtherStr
```

- **InstanceName**: is a string referring to one of the child nodes at the current level in the instance tree. Typically it is the unique name of one of the molecules you have instantiated, but it can also be the name of one of the atoms or bonded interactions within these molecules.

- **ObjectTypeName**: is a string that refers to the name of one of the child nodes at the current level in the static tree. That node typically refers to a type of molecule or a type of atom or bonded interaction, or an object containing force field information (like "TraPPE" or "OPLSAA").

- **CategoryName**: is a type of counter variable *category*. Typical categories are "@atom", "$atom", "@bond", "$bond", "@angle", etc... However user-created categories are also possible using the "category" command. (See below.) In principle, each category is associated with a node in the static tree (@) or instance tree ($) which limits the scope of the counter to children of that node. However in practice most categories (eg "@atom", "$bond", ...) are associated with the root node ("/") by default, and are thus global in scope. The syntax for creating custom categories and referring to them later is explained in appendix D.2.

- **FileName**: Strings refering to the names of files.

- **OtherStr**: Strings which do not fall into any of these categories

See appendix G.1 for details explaining the syntax of $ and @-style variables, including **CategoryNames** and node references.

Production Rules

Moltemplate LT files contain lists of commands.

```
CommandList ::= "" | Command CommandList
```

...where

```
Command ::= ObjectDef | InstanceCommand | DeleteCommand | WriteC | WriteOC |
            ImportCommand | CategoryDef | InstanceMod | ObjectTypeMod |
            ObjectDefMod | ReplaceCommand | UsingCommand | PushXform

ObjectDef ::= ObjectTypeName ClassParents "{" CommandList "}"
ClassParents ::= "" | "inherits" ParentList
ParentList ::= StaticNode | StaticNode ParentList
StaticNode ::= ObjectTypeName | ObjectTypeName "/" StaticNode

InstanceCommand ::= InstanceName "=" "new" InstanceExpr
InstanceExpr ::= InstanceName RangeNDX
RangeNDX ::= "" | RangeX RangeNDX
RangeX ::= "[" IntRange "]" Xforms
IntRange ::= Integer | Integer ":" Integer | "*"
Xforms ::= "" | Xform Xforms
Xform ::= MoveXform | RotXform | ScaleXform
MoveXform ::= ".move(" Number "," Number "," Number ")"
RotXform ::= ".rot(" Number "," Number "," Number "," Number ")"
ScaleXform ::= ".scale(" Number "," Number "," Number ")"
```

Deleting or modifying existing instances

```
InstanceMod ::= InstanceSelection XformsNE
DeleteCommand ::= "delete" InstanceSelection
InstanceSelection ::= InstanceNode RangeND
InstanceNode ::= InstanceName | InstanceNode "/" InstanceName
RangeND ::= "" | Range RangeND
Range ::= "[" IntRange "]"
XformsNE ::= Xform Xforms
```

Writing text containing counter variables

```
WriteC ::= "write(" FileName ")" "{" TemplateText "}"
TemplText ::= "" | String TemplText | StatVar TemplText | InstVar TemplText
InstVar ::= "$"CategoryName":"InstanceNode
StatVar ::= "@"CategoryName":"StaticNode

WriteOC ::= "write_once(" FileName ")" "{" TemplateTextStat "}"
TemplTextStat ::= "" | String TemplTextStat | StatVar TemplTextStat
```

Miscellaneous

```
ImportCommand ::= "import" FileName


ReplaceCommand ::= "replace" { StatVar StatVar }


CategoryCommand ::= CatCommandStat | CatCommandInst
CatCommandStat ::= "category" "@"CategoryName"(" Integer "," Integer ")"
CatCommandInst ::= "category" "$"CategoryName"(" Integer "," Integer ")"
```

```
ObjectTypeMod ::= ObjectTypeName XformsNE
ObjectDefMod ::= ObjectTypeName "=" ObjectTypeName XformsNE

UsingCommand ::= "using" "namespace" ObjectTypeName

PushXform := "push(" XformsNE ")" CommandList "pop()"
```

G.1 Counter variable syntax

Counter variables have names like:
    $**cpath**/**catname**:**lpath**
    or
    @**cpath**/**catname**:**lpath**
    (Note: All of the variable examples in this appendix can refer to either static @ variables or instance $ variables. Both variable types obey the same syntax rules. For brevity, only the instance $ variables are shown.)
    All counter variables have 3 parts:

> **cpath**, the category scope object (which is usually omitted)
>
> **catname**, the category name
>
> **lpath**, the "leaf path". This includes the variable's name and (optionally) the location of that variable in the object tree relative to the object in which the variable is referenced (the current-context object)

    Typically the **cpath** is omitted, in which case it means that the category has global scope. *(This is true for all of the standard counter variable types: "@atom", "$atom", "$mol", "@bond", "$bond", "@angle", "$angle", "@dihedral", "$dihedral", "@improper", and "$improper".)* However the **cpath** can be specified explicitly, as in this example: "$/atom:" ("/" denotes explicitly that the counter has global scope). Another example with an explicit **cpath** is the custom local counter variable named "$/proteins[5]/monomerid:." (See section D.3.) In this example, the **cpath** is "$/proteins[5]", the **catname** is "monomerid", and the **lpath** is ".". (In section D.3, we never explicitly specified the **cpath**. This is a source of confusion. When **cpath** is omitted, then the program searches up the tree for an ancestor node containing a category with a matching **catname**. Consequently the **cpath** rarely ever needs to be stated explicitly. See section G.3 for more details.)

G.2 General variable syntax

The ellipsis ("...") commonly appears in counter variables (or it is implied). The most complex and general variable syntax is:
    $**cpath**/.../ **catname**:**lpath**
    This means: find the closest ancestor of the **cpath** object containing a category named "**catname**". This ancestor determines the category's

scope. Counter variables in this category are local to ancestors of that object. In this usage example, *lpath* identifies the location of the variable's corresponding "leaf" object relative to the category scope object (*cpath*). On the other hand, if the the category's scope (*cpath*) was not explicitly stated by the user (which is typical), then the *lpath* identifies the location of the leaf object relative to the object in which the variable was referenced (the current-context ".").

G.3   Variable shorthand equivalents

$*catname*:*lpath* is equivalent to "$.../*catname*:*lpath*"

This means: find the closest direct ancestor of the current object containing a category whose name matches *catname*. If not found, create a new category (at the global level). *This is the syntax used most frequently in LT files.*

If the colon is omitted, as in $*lpath*/*catname*, then it is equivalent to: $*catname*:*lpath*. Again, in these cases, *lpath* is a path which is relative to the object in which the variable was referenced.

If $*lpath* is omitted, then this is equivalent to $*catname*:. In other words, the the leaf node is the current node, ".". (This syntax is often used to count keep track of molecule ID numbers. You can use the counter variable "$mol" to keep track of the current molecule id number, because it counts the molecular objects in which this variable was defined. In this case the name of the category is "mol". As in most examples, the category object, *cpath*, is not specified. This means the category object is automatically global. A global category object means that every molecule object is given a unique ID number which is unique for the entire system, not just unique within some local molecule. As a counter-example, consider amino acid residue counters. Each amino acid in a protein can be assigned a residue ID number which identifies it within a single protein chain. However because their category was defined locally at the protein level, these residue ID numbers are not global, and are not uniquely defined if there are multiple protein chains present.) (See section D.3 for details.)

$*cpath*/*catname*:*lpath*/...

(SHORTHAND equivalent)

Find the category name and object corresponding to "$*cpath*/*catname*:" (see above) If $*cpath*/ is blank, then search for an ancestor with a category whose name matches *catname*, as described above. To find the variable's corresponding "leaf object", start from the CURRENT object (not the category object). If *lpath* is not empty, follow *lpath* to a new position in the tree. Otherwise, start at the current object. (An empty *lpath* corresponds to the current object.) From this position in the object tree search for a direct ancestor which happens to also be "leaf object" for some other variable which belongs to the desired category. If no such variable is found, then ttree creates a new variable whose leaf object is the object at the *lpath* position, and put it in the desired category.

$*lpath*/.../*catname* **is equivalent to** **$*catname*:*lpath*/...**

(SHORTHAND equivalent)

If ***lpath*** is omitted, then start from the current node. (In the molecular examples, "$.../mol" is a variable whose category name is "mol". The "leaf object" for the variable is either the current object in which this variable was defined, OR a direct ancestor of this object which has been assigned to a variable belonging to the category named "mol". In this way large objects (large molecules) can be comprised of smaller objects, without corrupting the "mol" counter which keeps track of which molecule we belong to. In other words, "$.../mol" unambiguously refers to the ID# of the large molecule to which this sub-molecule belongs (regardless of however many layers up that may be).)

$*cpath*/*catname*:*lpath*

Variables in the output_ttree/ttree_assignments.txt file use the this syntax.

If the user explicitly specifies the path leading up to the cat node, and avoids using "...", then ***lpath*** is interpreted relative to the category object, not the current object (however ***cpath*** is interpreted relative to the current object). This happens to be the format used in the "ttree_assignments.txt" file (although you can use it anywhere else in an ".LT" file). In "ttree_assignments.txt" file, ***cpath*** is defined relative to the global object. The variables in that file always begin with "$/" or "@/". The slash at the beginning takes us to the global environment object (to which all the other objects belong). (Since the variables in the "ttree_assignments.txt" always begin with "$/" or "@/", this distinction is usually not important because the category object for most variables usually is the "global" root object.)

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