10.1.3 Advanced graphics features in the *dump image* command

Added in version TBD.

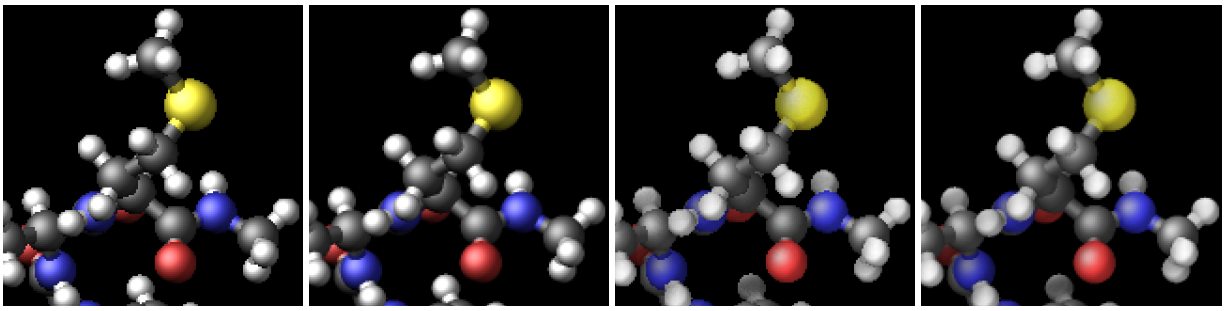
The following paragraphs discuss some of the more advanced features in the *dump image* command in LAMMPS with the help of some simple input file examples. For exact details of keywords and arguments, please refer to the detailed documentation of the command.

Please note that many of these features were added or significantly updated after LAMMPS version 10 Sep 2025 and well into the 2026 stable version development cycle. If you are using an older version of LAMMPS, these examples will cause errors or may look differently.

Available topics

Image quality and resolution

The two keywords *fsaa* and *ssao* can be used to improve the image quality at the expense of additional computational cost to render the images. The images below show from left to right the same render with the default settings, with *fsaa* enabled, with *ssao* enabled, and with both features enabled.



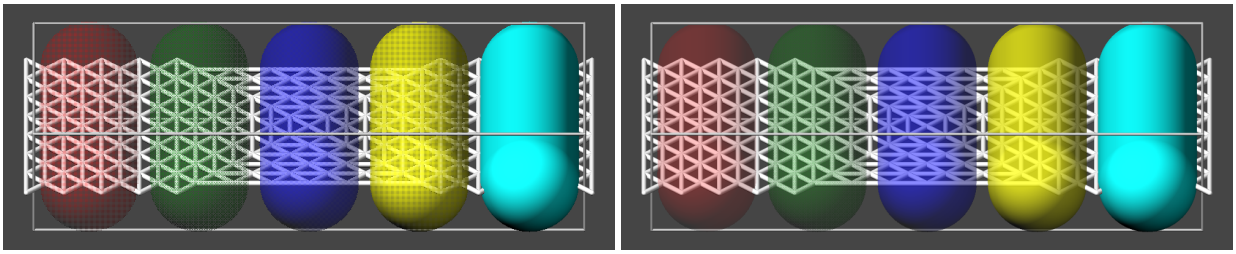
The computational cost to create the images with *dump image* depends on the image size, the number of objects to be rendered (this number can grow quickly when using fine triangle meshes), and the choice of the *fsaa* and *ssao* settings. For high resolution images, a correspondingly large image size has to be chosen. Same as it is done implicitly when enabling FSAA, one can improve image quality by rendering images at a large size and then processing and scaling

them to the desired size in a image processing software. Since the simulation has to wait for dump image to complete its image rendering, creating high resolution and high quality images can slow down as simulation significantly. On the other hand, the image rasterizer in LAMMPS is fairly simple and thus fast compared to more advanced image generation tools like ray tracers. At the moment there is no GPU acceleration or multi-threading parallelization available, except for the multi-threading support for SSAO processing.

Transparency

It is now possible to create approximately transparent graphics objects using an ordered dithering algorithm which results in a so-called *screen-door transparency* effect. In essence, for a transparent object only a part of the pixels are drawn and thus exposing any object behind the transparent object where drawing the pixels is skipped. LAMMPS employs a 16x16 Bayer matrix pattern that leads to rather regular patterns. A benefit of this approach is that it does not add extra cost to the rendering and for a 25%, 50%, and 75% transparency setting, there are no visible pixel patterns when also FSAA is enabled. In this case each pixel is the average of a 2x2 block of pixels in an image of double the width and height, and thus the transparent object will contribute 3, 2, or 1 pixels to the 2x2 block which is averaged.

Transparency is typically - like the color of objects - associated with an atom type and can be modified through the *dump_modify atrans* command and specified as an opacity ratio, i.e. a number between 0 (fully transparent) and 1 (fully opaque). Other choices are available and described in the documentation page.



Creating and viewing animated GIFs and movie files

A series of JPEG, PNG, or PPM images can be converted into a movie file and then played as a movie using commonly available tools. Using dump style *movie* automates this step *and* avoids the intermediate step of writing (many) image snapshot file. But LAMMPS has to be compiled with `-DLAMMPS_FFMPEG` and a compatible FFmpeg executable has to be installed. When using LAMMPS-GUI to run LAMMPS, you can run the simulation and LAMMPS-GUI will automatically show the created images in its `Slideshow Viewer` dialog. From there you can animate or single step through them and also export them to a movie file via FFMpeg.

To manually convert JPEG, PNG or PPM files into an animated GIF or MPEG or other movie file you can use:

1. Use the ImageMagick `convert` program (called `magick` in recent versions).

   ```
   convert *.jpg foo.gif
   convert -loop 1 *.ppm foo.mpg
   ```

   Animated GIF files from ImageMagick are not optimized. You can use a program like gifsicle to optimize and thus massively shrink them. MPEG files created by ImageMagick are in MPEG-1 format with a rather inefficient compression and low quality compared to more modern compression styles like MPEG-4, H.264, VP8, VP9, H.265 and so on.

2. Use QuickTime.

   Select "Open Image Sequence" under the File menu Load the images into QuickTime to animate them Select "Export" under the File menu Save the movie as a QuickTime movie (*.mov) or in another format. QuickTime

can generate very high quality and efficiently compressed movie files. Some of the supported formats require to buy a license and some are not readable on all platforms until specific runtime libraries are installed.

3. Use FFmpeg

   FFMpeg is a command-line tool that is available on many platforms and allows extremely flexible encoding and decoding of movies.

```
cat snap.*.jpg | ffmpeg -y -f image2pipe -c:v mjpeg -i - -b:v 2000k movie.m4v
cat snap.*.ppm | ffmpeg -y -f image2pipe -c:v ppm -i - -b:v 2400k movie.mp4
```

   Front ends for FFmpeg exist for multiple platforms. For more information see the FFmpeg homepage

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Play the movie:

1. Use your web browser to view an animated GIF or MP4 movie format movie.

   Select "Open File" under the File menu Load the animated GIF or MP4 movie file

2. Use the freely available VideoLAN media player (vlc) or FFMpeg player tool (ffplay) to view a movie.

   Both are available for multiple operating systems and support a large variety of file formats and decoders. There are plenty more media player packages available on the different operating systems.

```
vlc foo.mpg
ffplay bar.avi
```

3. Use the Pizza.py animate tool, which works directly on a series of image files.

```
a = animate("foo*.jpg")
```

4. QuickTime and other Windows- or macOS-based media players can obviously play movie files directly. Similarly for corresponding tools bundled with Linux desktop environments. However, due to licensing issues with some file formats, the formats may require installing additional libraries, purchasing a license, or may not be supported.

Visualizing systems using potentials with implicit bonds

There are several pair styles available in LAMMPS where the bond information is not taken from from the bond topology in a data file but the potentials first determine a "bond-order" parameter for pairs of atoms and - depending on the value of that parameter - apply forces for bonded interactions. This applies to *ReaxFF*, *REBO and AIREBO*, *BOP*, and several others pair styles. These implicit bonds will not be shown by *dump image* since its mechanism for displaying bonds relies on explicit bonds being present in the bond topology.

One can hide the fact that there are no bonds by setting the atom radii to the covalent radii of the corresponding elements (see leftmost example image below). This will result in a representation often labeled as "VDW" in popular visualization tools. Otherwise, there are currently three approaches to make those bonds visible.

1. Access the (internal) bond order information from the pair style through a custom fix and then use the *fix* keyword of the *dump image* command to use the graphics objects information provided by the fix to visualize the bonds (see below for more information). That includes bonds that are broken and formed. This is the most accurate option since it uses the data that is used by the computation of the model. This is currently only available for ReaxFF by using *fix reaxff/bonds*.

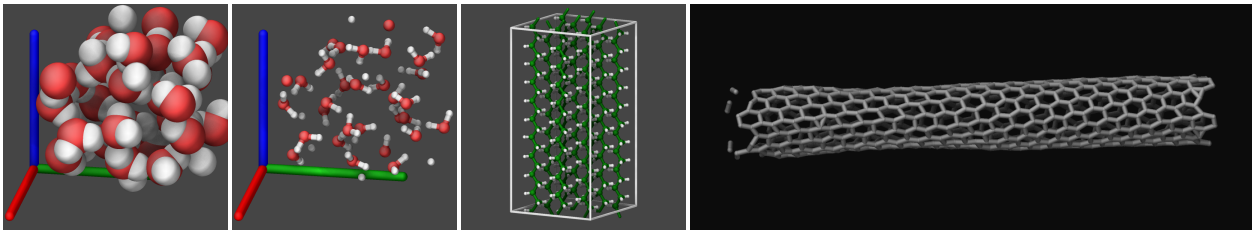
   #. Use the *autobonds* keyword of *dump image* to approximate the bonds based on a simple distance heuristic. This is similar to the *Dynamic Bonds* representation in VMD. How accurate this option will be depends on the complexity of the system and how many different bond lengths there are. For the simple water system shown

below, there are no significant differences, since there is only one type of bond (between oxygen and hydrogen). The *autobond* keyword uses on top of the distance cutoff between atoms, the heuristic that no bonds will be drawn between two hydrogen atoms and thus bogus bonds are avoided when using a larger bond cutoff (e.g. suitable for carbon-carbon bonds) which is larger than the typical hydrogen-hydrogen distance for hydrogen atoms bound to the same atom (e.g. in water, methane or hydrocarbon chains).

2. Use use a combination of *fix bond/break* and *fix bond/create/angle* with *bond style zero* to dynamically create and remove bonds that do not add any forces. This also requires to tell the neighbor list code to not treat any pairs of atoms as special neighbors (otherwise the corresponding pairs of atoms could be excluded from the neighbor list and thus the forces computed by the pair style incorrect) through using the *special_bonds* command. Unlike the two other options which were recently added when this document when was written, this method also works with older versions of LAMMPS. Here is an example of the necessary commands for a carbon nanotube (that is modeled with AIREBO):

```
bond_style zero
bond_coeff 1 1.4
special_bonds lj/coul 1.0 1.0 1.0
fix break all bond/break 1000 1 2.5
fix form all bond/create/angle 1000 1 1 2.0 1 aconstrain 90.0 180
```

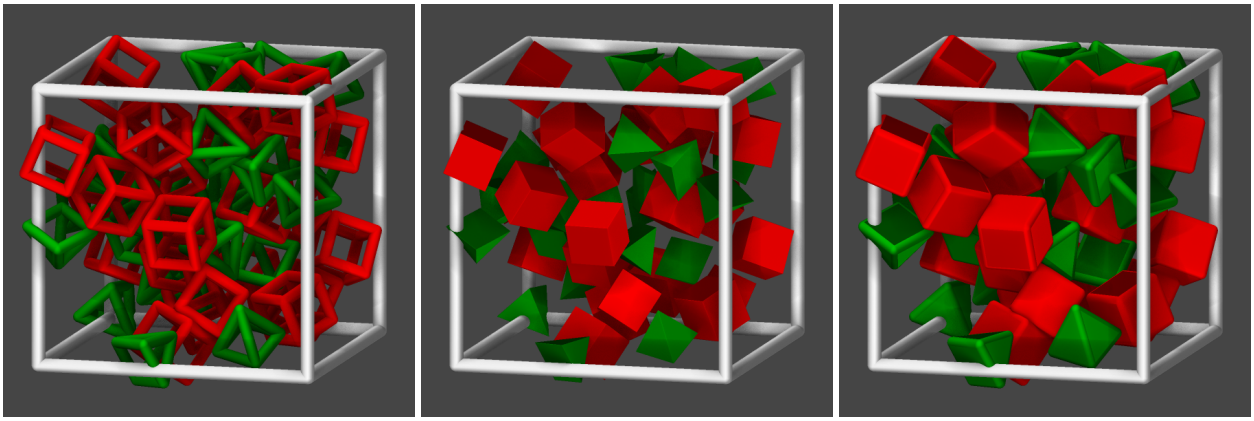
This "graphics hack" was originally posted as part of the LAMMPS tutorial at https://lammpstutorials.github.io/sphinx/build/html/tutorial2/breaking-a-carbon-nanotube.html



Visualizing body particles

Body particles are objects formed from either a collection of spherical particles, polygons (in 2d), or polyhedra (in 3d) formed from triangular or quadrilateral surfaces. The regular *dump* command can only output the center of those bodies (and their orientation), which complicates the visualization with external tools. In addition, the position of the constituent particles of *nparticles* bodies or the positions of the vertices of *rounded/polygon* or *rounded/polyhedron* bodies, which can be computed with *compute body/local* and output with *dump local*.

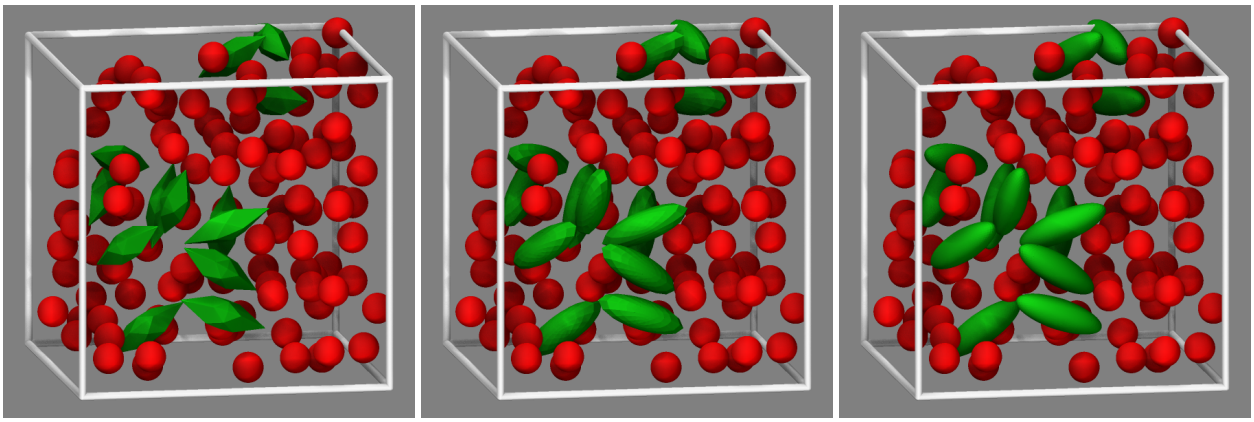
As an alternative, the bodies can be visualized directly with *dump image* using the *body* keyword. Without the *body* keyword the body particles would be visualized like atoms as single spheres. The color and transparency settings can be changed by settings those properties for the corresponding atom types. It is also possible to represent the bodies as either wireframes (*bflag1* value 2), planar faces (*bflag1* value 1), or both (*bflag1* value 3).



Visualizing ellipsoid particles

Ellipsoidal particles are a generalization of spheres that may have three different radii to define the shape. They can be modeled using pair styles *gayberne* or *resquared*. The regular *dump custom* command can output the center of those bodies, the shape parameters and the orientation as quaternions. If one follows the required conventions and follows the documented steps, those trajectory dump files can be imported and visualized in OVITO

As an alternative, the ellipsoid particles can be visualized directly with *dump image* using the *ellipsoid* keyword. The color and transparency settings can be changed by settings those properties for the corresponding atom types. It is also possible to represent the ellipsoids via generating a triangle mesh and visualizing it as either wireframes (*eflag* value 2), planar faces (*eflag* value 1), or both (*eflag* value 3), same as demonstrated for body particles above. The use of a triangle mesh is currently required since the rasterizer built into LAMMPS does not offer a suitable graphics primitive for ellipsoids. The mesh is constructed by iteratively refining a triangle mesh representing an octahedron where each triangle is replaced by four triangles. For a smooth representation a refinement level of 5 or 6 is required, which will cause a significant slowdown of the rendering of the image. Also, some artifacts can happen due to rounding which can be somewhat minimized using FSAA (which causes further slowdown of the rendering).



These images were created by adding the following *dump image and dump_modify* commands to the `in.ellipse.resquared` input example:

```
#                                                  change + this
dump viz all image 1000 image-*.png type type ellipsoid type 3 4 0.05 &
      size 600 600 zoom 2.2 shiny 0.1 fsaa yes view 80 -10 box yes 0.025 &
      axes no 0.0 0.0 center s 0.5 0.5 0.5 ssao yes 32185474 0.6
dump_modify viz pad 9 boxcolor white backcolor gray adiam 1 4 adiam 2 7
```

Visualizing regions

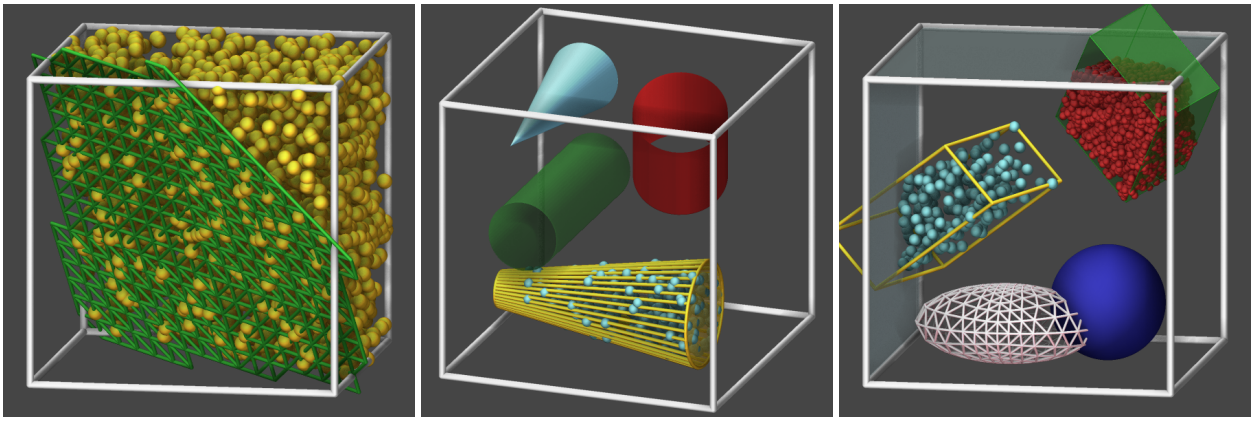
Since there are several commands that operate on atoms within a specific *region* , it can be helpful to visualize the extent of those regions, either for debugging the command settings or for visualizing the production simulation. This is even more useful when regions are (dynamically) translated or rotated or both with the *rotate* or *move* keyword of the *region* command. The *dump image region* keyword can be used to enable such visualizations. There are currently four different draw styles available:

- *filled*: a mesh of triangles is constructed for the surface of the region and then drawn in the selected color. This draw style accounts for the *open* keyword of the *region* command and only draws the faces of a region that are closed.
- *transparent*: this is the same visualization as draw style *filled*, but in addition one can set the transparency of that visualization through an opacity parameter in the range of 0.0 (invisible) to 1.0 (fully opaque).
- *frame*: uses the same mesh of triangles as the two styles above above, but renders the region's surface as a wireframe mesh with a given cylinder diameter.
- *points*: generates a cloud of random points inside the simulation box and then only draws a point as a sphere with the given color and radius if it is located inside the region. This is useful to check the impact of the *side in/out* setting of a region, and complementary to the other three draw styles, which only show the region surfaces. For visualization purposes any open faces of a region are ignored, since a region with an open face matches *all* particles.

It can sometimes be convenient to draw the same region with multiple draw styles as can be seen from the example visualization images below.

Notes on the visualization of individual region styles:

- *plane*: since in theory planes extend infinitely, some form of boundary has to be established for the visualization. Therefore a mesh of triangles is constructed and transformed according to the region settings and then only those triangles are drawn, where at least one corner is inside the simulation box. For draw style *points* the *side in/out* setting determines on which side of the plane the points are drawn.
- *cone* and *cylinder*: use triangle meshes for draw styles *filled* and *transparent* since there are no equivalent primitives (the cylinder primitive only draws half of the cylinder, since it is optimized for being capped). For draw style *frame*, only the rim of the top or bottom is drawn and the side is represented by lines from the top to the bottom.
- *box* and *prism*: for draw style *frame* only the edges of the region are shown; for draw styles *filled* and *transparent*, the faces are drawn instead, but only if they are not set as "open" in the *region* command.



Below is an example input deck for visualizing *cone* and *cylinder* regions:

```
region      box block -2 2 -2 2 -2 2
create_box 0 box

variable rot equal PI*step/1000.0

region c1 cylinder x -1.0 0.0 0.5 -1.5 1.5 open 1 open 2
region c2 cone y  1.0 -1.0 0.25 0.75 -1.5 1.5 open 3
region c3 cylinder z  0.0 1.0 0.66 -0.1 1.5 open 1 open 2 rotate v_rot 0.3 0.0 0.3 0.0 1.
↪0 1.0
region c4 cone x -1.0 1.5 0.5 0.0 -1.0 2.0

dump viz all image 100 image-*.png type type size 600 600 zoom 1.4 shiny 0.1 view 70 20 &
             box yes 0.025 axes no 0.0 0.0 fsaa yes ssao yes 314123 0.7 &
             region c1 forestgreen transparent 0.5 &
             region c2 goldenrod frame 0.05 &
             region c2 cadetblue points 10000 0.15 &
             region c2 goldenrod transparent 0.5 &
             region c3 firebrick filled &
             region c4 skyblue filled
dump_modify viz pad 4 boxcolor silver backcolor darkgray

run 500
```

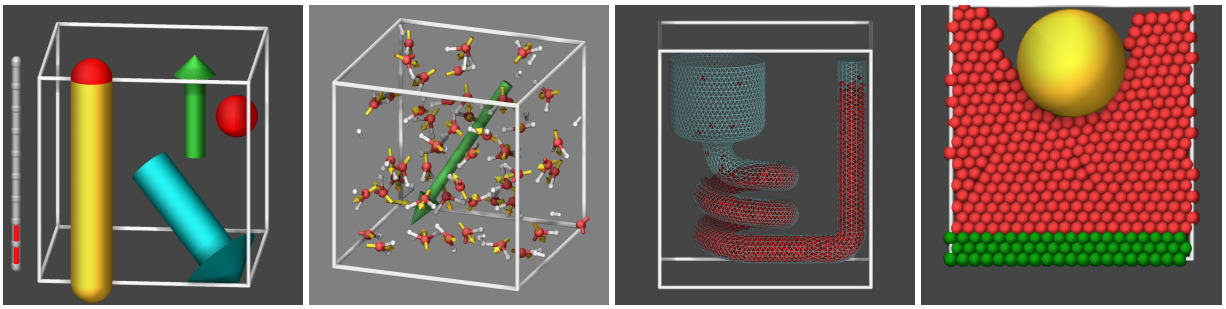
Visualizing graphics provided by fix commands

LAMMPS can display additional graphics objects in the *dump image* output that are added by fix styles. These fall in two categories: fixes that were written with the specific purpose of adding graphics to the visualization and fixes that make objects or data visible that they maintain internally. Examples for the latter case are visualizing the indenter object from *fix indent* or the wall position from one of the wall fixes. The details of what kind of graphics is added and how it can be configured is described in a section titled **Dump image info** in the documentation of the individual fix commands.

Below is a table with links to the documentation of supported fix styles:

fix graphics	*fix graphics/arrows*	*fix indent*	*fix reaxff/bonds*
fix smd/wall_surface	*fix wall/lj93*	*fix wall/lj126*	*fix wall/lj1043*
fix wall/colloid	*fix wall/gran*	*fix wall/harmonic*	*fix wall/harmonic/outside*
fix wall/lepton	*fix wall/morse*	*fix wall/reflect*	*fix wall/reflect/stochastic*
fix wall/table			

There is no support for *fix wall/region* and *fix wall/gran/region*, since regions can be visualized with the *region* keyword of *dump image* already (see discussion above).



Below are discussions about some aspects of specific fix commands and some input examples.

Fix graphics

Fix *graphics* adds some graphics primitives and more complex objects like a progress bar to the visualization where properties of the object(s) are controlled by *equal-style or compatible variables*.

Fix graphics/arrows

Fix *graphics/arrows* adds per-atom or per-chunk arrows to the visualization. The arrows represent some per-atom property or per-chunk 3-vector property. For atoms, there are the pre-defined properties *force*, *velocity*, and *dipole*. Everything else would have to be computed in *atom-style or compatible variables*. For per-chunk properties, one needs to provide the IDs of three computes: a *chunk/atom compute* and two per-chunk computes where the first defines the position of the (middle of the) arrow and the second the direction and length of the arrow. Popular choices would create per-molecule or per-bin chunks. Below is an example input section that computes and displays both, the total dipole moment (using *fix graphics* and the per-molecule dipole moment as arrows in addition to the per-atom velocities:

```
compute molchunk all chunk/atom molecule
compute cpos all com/chunk molchunk wrap yes
compute cdip all dipole/chunk molchunk
fix vel all graphics/arrows 10 velocity 50.0 0.066 autoscale 0.25
fix vec all graphics/arrows 10 chunk molchunk cpos cdip 3 0.1

compute dip all dipole
variable scale equal 0.75
variable dip1x equal -v_scale*c_dip[1]
variable dip1y equal -v_scale*c_dip[2]
variable dip1z equal -v_scale*c_dip[3]
variable dip2x equal v_scale*c_dip[1]
variable dip2y equal v_scale*c_dip[2]
variable dip2z equal v_scale*c_dip[3]
fix dipole all graphics 1 arrow 1  v_dip1x v_dip1y v_dip1z v_dip2x v_dip2y v_dip2z 0.3 0.
↪2

dump viz all image 100 image-*.png element type size 600 600 zoom 1.3 view 70 20 shiny 0.
↪1 &
             bond atom 0.2box yes 0.025 axes no 0.0 0.0 center s 0.5 0.5 0.5 fsaa yes &
             fix dipole const 0 0 fix vec const 0 0 fix vel const 0 0 ssao yes 315465 0.8
dump_modify viz pad 6 boxcolor white backcolor gray element O H  bdiam 1 0.2 &
             adiam 1 0.5 adiam 2 0.3 acolor 1 silver acolor 2 red fcolor vec goldenrod &
             fcolor dipole forestgreen ftrans dipole 0.75 fcolor vel cyan ftrans vel 0.5
```

Fix reaxff/bonds

Fix *reaxff/bonds* of the *REAXFF package* provides access to the list of bonds as they are dynamically computed by the *ReaxFF pair style*. As discussed above, this can be used to visualize bonds for a system where there is no explicit bond topology defined.

Fix smd/wall_surface

Fix *smd/wall_surface* of the *MACHDYN package* creates a custom wall from a mesh of triangles that is read from an STL format file.