NAME

asphere_vis - Tools for ellipsoid visualization in PyMol of a LAMMPS trajectory.

VERSION

Version 0.2

SYNOPSIS

asphere_vis flavor_file dump_file output_py_file [**-b**] [**-f** *max_frame*] [**-h**] [**-i** *start_frame skip end_frame*] [**-n** *notice_level*] [**-o**] [**-r** *ellip_res*] [**-s**]

DESCRIPTION

Tool for converting LAMMPS trajectories into compiled graphics objects for visualization in PyMol. The *flavor_file* is an input file that describes the color, transparency, and size/shape of each atom type. The *flavor_file* consists of two possible line formats. For spherical particles, the format is:

atom_type color alpha diameter

where alpha is used to adjust the transparency of the particle. For ellipsoidal particles, the format is:

atom_type color alpha diameter_x diameter_y diameter_z

Ellipsoidal and spherical line formats can be mixed in the same *flavor_file* For any atom type not listed in the *flavor_file* a blue sphere of size 1 is assumed.

The *dump_file* is a LAMMPS trajectory. For atom types specified as spherical in the *flavor_file*, the *dump_file* must contain *tag type x y z* as the first columns. For atom types specified as ellipsoidal in the *flavor_file*, the columns are *tag type x y z quatw quati quatj quatk*.The latter can be gerenated, for example, with the LAMMPS dump_style custom command with the following arguments in order:

tag type x y z quatw quati quatj quatk

The output file is a python file for input to Pymol. This can be viewed from the command line using *pymol output.py* or by using the *run* command from within Pymol.

PARAMETERS

-b When used with **-s**, the option will number the filenames based on the frame number. By default, they are numbered consequtively from zero.

-f *max_frame*

Do not write more than *max_frame* frames to the output file.

-h Print out the man page for help

-i *start_frame skip end_frame*

Render the specified frame interval inclusive between *start_frame* and *end_frame*. *skip* gives the number of frames to *skip* between each rendered frame. A value of 0 outputs every frame between *start_frame* and *end_frame*. The first frame in the dump file is frame 0.

-n *notice_level*

Set the degree of program output. Use:

-n 0 No output
-n 10 Normal program output
-n 20 Parameters useful for reproducing the results
-n 30 All output

-o Do not output the outline for the simulation box.

-r *ellip_res*

Resolution of ellipsoids in PyMol. The number of triangles per ellipsoid is equal to 2*(*ellip_res*^2). Default is 10.

-s Output the results into separate .py files. The filename and extension for the output files is taken from *output_py_file*.

AVAILABLE COLORS

black
blue
brown
cmyk_blue
cmyk_marine
deep
forest
green
grey
hotpink
magenta
marine
orange
purple
red
slate
teal
wheat
white
yellow

AUTHORS

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