NAME

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

VERSION

Version 0.1

SYNOPSIS

asphere_vis input_file dump_file output_py_file [**-b**] [**-c** *color_file*] [**-d**] [**-f** *max_frame*] [**-h**] [**-i** *start_frame skip end_frame*] [**-n** *notice_level*] [**-r** *ellip_res*] [**-s**]

DESCRIPTION

Tool for ellipsoid visualization in PyMol of a LAMMPS trajectory. The *input_file* is a LAMMPS data file with a 'Shapes' section or a LAMMPS input script file with ellipsoid diameters specified using the 'shape' command. The trajectory is input from *dump_file* that must be generated using a LAMMPS dump_style custom command with the following arguments in order:

tag type x y z quatw quati quatj quatk

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.

-c *color_file*

Color the atom_types and set transparency based on the color file. The color file contains a space delimited set sequence of the color for an atom followed by the alpha. The color should be the string name and the alpha should be between 0 and 1.

-d   Use a LAMMPS input script rather than a data file for extracting atom shape information. The input script is specified as *input_file*.

-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

-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

KNOWN BUGS
Comments are not allowed at any point between a section header and the end of the contents for a section in either the data file or the input file.

AUTHORS
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