NAME

asphere_vis - Tools for LAMMPS ellipsoid trajectory visualization in PyMol.

VERSION

Version 0.1

SYNOPSIS

asphere_vis input_data_file input_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 LAMMPS trajectory visualization in PyMol. The input is a LAMMPS 'data' file or a 'in' file with ellipsoid semi-axes specified using the ellipsoid command. The trajectory is input from a 'dump' file that must be generated using a custom style 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 input file. The input 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 file rather than a data file for extracting atom type information. The input filename is specified as *input_data_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 trajectory. 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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