fix ext_alignment

Release 0.1

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CONTENTS:

CHAPTER

ONE

SYNTAX

```
fix ID group-ID ext_alignment particle_axis fdx fdy fdz force_constant
```

- ID, group-ID are documented in fix command
- ext_alignment = style name of this fix command
- particle_axis = *angle_f* or *angle_v* or *angle_u*
- fdx,fdy,fdz = external field component values (distance units)
- force_constant = alignment force constant magnitude (force units)

CHAPTER

TWO

EXAMPLES

```
fix torque all ext_alignment angle_u 1 1 0 90.0
fix torque crystals ext_alignment angle_v 0 1 0 150.0
fix field polymer ext_alignment angle_u 0 0 1 1000.0
```

CHAPTER

THREE

DESCRIPTION

Add a torque to a specified axis of a particular group of finite-size particles with respect to a fixed direction. The applied torque is as follows:

$$\tau = \begin{cases} k(\hat{u}_i \times \hat{\psi}), & \text{if} \hat{u}_i \cdot \hat{\psi} > 0 \\ -k(\hat{u}_i \times \hat{\psi}), & \text{if} \hat{u}_i \cdot \hat{\psi} < 0 \end{cases}$$

were k is the force constant that determines how aggressive is the external alignment field, $\hat{u}_i$ is the axis of the finite-size particle to be aligned with respect to the direction of the external field, and $\hat{\psi}$ is the unit directional vector. The direction of $\hat{\psi}$ can be set in any direction of a fixed 3D space. This torque allows a parallel alignment of the particles with respect to the field, regardless of whether their main axis ($\hat{u}_i$) is pointing in the opposite direction as $\hat{\psi}$.

This command can be used to induce an artificial alignment to finite-size particles in a simulation, such as for liquid crystal simulations of uniaxial or biaxial particles.

particle_axis assumes that the orientation of each site in the specified group-ID is given by an orthonormal basis ($\hat{f}$, $\hat{v}$, $\hat{u}$), and therefore one must specify the direction to be oriented.

External field component values can take any desired values since they are normalized in the code, but it is suggested to use numbers from 0 to 1.

Note that this fix can only act on finite-size particles. Therefore, there must be an Ellipsoids section in the LAMMPS input to obtain the orientation of the particles. See atom_style command ellipsoid.

CHAPTER

FOUR

RESTART, OUTPUT, RUN START/STOP

No information about this fix is written to binary restart files.

No parameter of this fix can be used with the start/stop keywords of the run command.

CHAPTER

FIVE

RESTRICTIONS

This fix does not support equal-style or atom-style variable.

Particles acted on by the potential can be finite-size aspherical or spherical particles.

This fix is only enabled if LAMMPS was compiled with fix_ext_alignment.cpp and fix_ext_alignment.h.

Note: This fix is currently supported in the latest LAMMPS stable release 23 Jun 2022. See the LAMMPS website for more info.

CHAPTER

SIX

RELATED COMMANDS

fix addforce, fix efield

CHAPTER

SEVEN

DEFAULT

none