The fix keyword

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Purpose

- This keyword is used to fix (freeze) a group of atoms

Grammar

- This keyword requires a single parameter which is the label of the group in which the atoms are to be fixed (velocities and forces are always set to zero such that the atoms in the group do not move). The full command reads

```
fix group_label
```

Here, the `group_label` refers to the grouping method 0 defined in the `xyz.in` file.

Examples

- We will illustrate the usage of this keyword in a Tutorial: Thermal transport from NEMD and HNEMD.

Caveats

- This keyword is not propagating, which means that it only affects the simulation within the run it belongs to.

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