

[WIP] LAMMPS support #319



Open jhprinz wants to merge 24 commits into `openpathsampling:master` from `jhprinz:lamps`



Conversation 12

Commits

24



Checks 0



Files changed 7



jhprinz commented on Oct 5, 2015

Member



This is part of future stuff, but I thought to give it a little try. Apparently there is a python API for lammps that could make all of this extremely simple. [LAMMPS Python Docs](#)

So far no luck in installing LAMMPS but I will figure it out eventually...



jhprinz added this to the **Future** milestone on Oct 5, 2015



first lammps engine running

✗ d53d16d



jhprinz commented on Oct 7, 2015

Member



Woohoo... Created an engine today. Seems that it is not so difficult to use our framework at all...

I ran a 1000 steps trajectory of a simple LJ Fluid for testing. Still some subtleties to figure out, but we might interest a lot of people once lammps is supported. Not sure how to really test this since I have so clue on how to properly use lammps... Means we might need someone that has used lammps before.

Demo!