Instructions for Installing LAMMPS, and Running a Granular Simulation

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Installing LAMMPS: I first describe the steps for building and compiling a public-release version of LAMMPS and its additional packages that are needed for running the simulations in the paper titled "A granular physics-based view of fault friction experiments" by Ferdowsi & Rubin. These instructions are suitable for installing and running LAMMPS on a UNIX or macOS machine. The version of LAMMPS used for running the simulations of this paper is "7Aug19", and it can be downloaded from LAMMPS webpage at https://lammps.sandia.gov/tars/. After downloading the code, choose a destination folder for installing the code (e.g., /home/username/Programs/ is used here), and copy the file "lammps-7Aug19.tar" there. Next, decompress "lammps-7Aug19.tar", and run the following commands in a terminal window to build the code:

Listing 1: Compiling LAMMPS on the cluster/computer

```
cd lammps-7Aug19/src
make mpi #builds the package in parallel form
```

The second command compiles a basic installation of LAMMPS with the option of parallel computing (using many computer cores to run simulations). The compilation may take a few minutes. When it is completed, you will see an output similar to the line below, which means that the MPI (Message Passing Interface) executable object has been built successfully:

```
make[1]: Leaving directory `/home/username/Programs/lammps-7Aug19/src/Obj_mpi'
```

For building and running the model described in this paper, we also need the following packages of LAMMPS: GRANULAR, USER-MISC, and RIGID. You can add these three packages to the basic installation of LAMMPS with the following commands in Programs/lammps-7Aug19/src:

Listing 2: Adding some additional packages to basic LAMMPS

```
make yes-user-misc  # adds the user-misc package to the basic build of LAMMPS
make yes-granular # adds the granular package to the basic build of LAMMPS
make yes-RIGID # adds the RIGID package to the basic build of LAMMPS
make mpi #builds the package in parallel form
```

Each of these commands should produce an output similar to the initial building, which indicates a new executable has been built successfully:

```
make[1]: Leaving directory `/home/username/Programs/lammps-7Aug19/src/Obj_mpi'
```

The LAMMPS installation for the purpose of running the simulations of this paper is complete. Further instructions for building the code is available at its webpage: https://lammps.sandia.gov/doc/Build.html.

Running LAMMPS Granular Simulations: You can run a LAMMPS simulation script (e.g., generation phase simulation, "generate_packing.bishear" script) with the following command:

Listing 3: Running a granular simulation with LAMMPS

```
mpirun -np [N] /home/username/Programs/lammps-7Aug19/src/lmp_mpi<generate_packing.
    bishear # this command runs the simulation script "generate_packing.bishear" on [N]
     cores. As an example, for running on N=4 cores, I give the command "mpirun -np 6 /
    home/username/Programs/lammps-7Aug19/src/lmp_mpi<generate_packing.bishear" without
    quotation marks. Replace "/home/username/Programs/" with LAMMPS parent directory
    address on your machine.
```

We have run the simulations for each grain size distribution and initial condition, in the order of (1) generating the fault gouge model ("generate_packing.bishear" script), (2) using the restart file from the generation phase to run the confinement phase simulation ("confine_granular_layer.bishear" script), and

(3) using the restart file from the confinement phase to run the shearing phase simulation ("shear_confined_granular_layer.bishear" script).