Running your first LAMMPS calculation:

1.) Open a terminal window and navigate to where you want output files (if any) to be placed

2.) Save the following text as “test.txt” on your computer (you’ll need the path to this file later)

```
# 3d Lennard-Jones melt

variable        x index 1
variable        y index 1
variable        z index 1
variable        t index 100

variable        xx equal 20*$x
variable        yy equal 20*$y
variable        zz equal 20*$z

units           lj
atom_style      atomic

lattice         fcc 0.8442
region          box block 0 ${xx} 0 ${yy} 0 ${zz}
create_box      1 box
create_atoms    1 box
mass            1 1.0

velocity        all create 1.44 87287 loop geom

pair_style      lj/cut 2.5
pair_coeff      1 1 1.0 1.0 2.5

neighbor        0.3 bin
neigh_modify    delay 0 every 20 check no

fix             1 all nve

thermo          100

# This is how you'd go to dump for VMD.  Dumps to running directory
dump myDump all xyz 1 test.xyz

run             $t
```

3.) Now in terminal input $ /path/to/your/build/of/LAMMPS -in /path/to/test.txt

Here is what I wrote on my machine:

/Users/kolbt/out_of_source_build_lammps/tmkolb-lammps/src/lmp_serial -in /Users/kolbt/desktop/test.txt