SURF Progress Meeting Document
Date : 9 / 18 / 2020

Wasn't able to work much on this the past week

Lots of different things came up

BMES
Capstone
Signals

+ More

Only able to Realy work on monday

Got a good 5 hours in then

Rest of week did bits and pisces of work

15 minutes here . 30 min there

Trying to Fix "fluidmembrane"

Trying to create "frankenstein" files

These are a combination of a working potential file (LJ Cut) and the non-working (fluidmembrane) files.

Tried to make these files and the initial C++ build worked, and I added the files (frankenstien.cpp and frankenstien.h) to the LAMMPS source code (as per the instructions) and Attempted to build LAMMPS

When trying to built LAMMPS however the build fails because of the 'Frankenstien" Files

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[ 10%] Building CXX object CMakeFiles/lammps.dir/home/jquinn/lammps/src/pair_morse.cpp.o
[ 10%] Building CXX object CMakeFiles/lammps.dir/home/jquinn/lammps/src/pair_soft.cpp.o
[ 10%] Building CXX object CMakeFiles/lammps.dir/home/jquinn/lammps/src/pair_table.cpp.o
[ 10%] Building CXX object CMakeFiles/lammps.dir/home/jquinn/lammps/src/pair_ufm.cpp.o
[ 10%] Building CXX object CMakeFiles/lammps.dir/home/jquinn/lammps/src/pair_yukawa.cpp.o
/home/jquinn/lammps/src/pair_fluidmembrane.cpp: In member function 'virtual void
LAMMPS_NS::Pairfluidmembrane::coeff(int, char**)':
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:220:44: error: no matching function for call to
'LAMMPS_NS::Force::bounds(char*&, int&, int&, int&)'
  220 |   force->bounds(arg[0],atom->ntypes,ilo,ihi);
      |                                            ^
In file included from /home/jquinn/lammps/src/pair_fluidmembrane.cpp:27:
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/home/jquinn/lammps/src/force.h:131:8: note: candidate: 'void LAMMPS_NS::Force::bounds(const char*,
int, char*, int, int&, int&, int)'
  131 |   void bounds(const char *, int, char *, int, int &, int &, int nmin=1);
      |        ^~~~~~
/home/jquinn/lammps/src/force.h:131:8: note:   candidate expects 7 arguments, 4 provided
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:221:44: error: no matching function for call to
'LAMMPS_NS::Force::bounds(char*&, int&, int&, int&)'
  221 |   force->bounds(arg[1],atom->ntypes,jlo,jhi);
      |                                            ^
In file included from /home/jquinn/lammps/src/pair_fluidmembrane.cpp:27:
/home/jquinn/lammps/src/force.h:131:8: note: candidate: 'void LAMMPS_NS::Force::bounds(const char*,
int, char*, int, int&, int&, int)'
  131 |   void bounds(const char *, int, char *, int, int &, int &, int nmin=1);
      |        ^~~~~~
/home/jquinn/lammps/src/force.h:131:8: note:   candidate expects 7 arguments, 4 provided
/home/jquinn/lammps/src/pair_fluidmembrane.cpp: In member function 'virtual void
LAMMPS_NS::Pairfluidmembrane::read_restart(FILE*)':
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:328:25: warning: ignoring return value of 'size_t
fread(void*, size_t, size_t, FILE*)', declared with attribute warn_unused_result [-Wunused-result]
  328 |       if (me == 0) fread(&setflag[i][j],sizeof(int),1,fp);
      |                    ~~~~~^~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:332:16: warning: ignoring return value of 'size_t
fread(void*, size_t, size_t, FILE*)', declared with attribute warn_unused_result [-Wunused-result]
  332 |         fread(&epsilon[i][j],sizeof(double),1,fp);
      |         ~~~~~^~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:333:16: warning: ignoring return value of 'size_t
fread(void*, size_t, size_t, FILE*)', declared with attribute warn_unused_result [-Wunused-result]
  333 |         fread(&sigma[i][j],sizeof(double),1,fp);
      |         ~~~~~^~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:334:16: warning: ignoring return value of 'size_t
fread(void*, size_t, size_t, FILE*)', declared with attribute warn_unused_result [-Wunused-result]
  334 |         fread(&cut[i][j],sizeof(double),1,fp);
      |         ~~~~~^~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:335:16: warning: ignoring return value of 'size_t
fread(void*, size_t, size_t, FILE*)', declared with attribute warn_unused_result [-Wunused-result]
  335 |         fread(&zeta[i][j],sizeof(double),1,fp);
      |         ~~~~~^~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:336:16: warning: ignoring return value of 'size_t
fread(void*, size_t, size_t, FILE*)', declared with attribute warn_unused_result [-Wunused-result]
  336 |         fread(&mu[i][j],sizeof(double),1,fp);
      |         ~~~~~^~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:337:16: warning: ignoring return value of 'size_t
fread(void*, size_t, size_t, FILE*)', declared with attribute warn_unused_result [-Wunused-result]
  337 |         fread(&beta[i][j],sizeof(double),1,fp);
      |         ~~~~~^~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
/home/jquinn/lammps/src/pair_fluidmembrane.cpp: In member function 'virtual void
LAMMPS_NS::Pairfluidmembrane::read_restart_settings(FILE*)':
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:376:10: warning: ignoring return value of 'size_t
fread(void*, size_t, size_t, FILE*)', declared with attribute warn_unused_result [-Wunused-result]
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  376 |     fread(&cut_global,sizeof(double),1,fp);
      |     ~~~~~^~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
[ 11%] Building CXX object CMakeFiles/lammps.dir/home/jquinn/lammps/src/pair_zbl.cpp.o
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:377:10: warning: ignoring return value of 'size_t
fread(void*, size_t, size_t, FILE*)', declared with attribute warn_unused_result [-Wunused-result]
  377 |     fread(&offset_flag,sizeof(int),1,fp);
      |     ~~~~~^~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
/home/jquinn/lammps/src/pair_fluidmembrane.cpp:378:10: warning: ignoring return value of 'size_t
fread(void*, size_t, size_t, FILE*)', declared with attribute warn_unused_result [-Wunused-result]
  378 |     fread(&mix_flag,sizeof(int),1,fp);
      |     ~~~~~^~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
[ 11%] Building CXX object CMakeFiles/lammps.dir/home/jquinn/lammps/src/pair_zero.cpp.o
make[2]: *** [CMakeFiles/lammps.dir/build.make:4295:
CMakeFiles/lammps.dir/home/jquinn/lammps/src/pair_fluidmembrane.cpp.o] Error 1
make[2]: *** Waiting for unfinished jobs....
/home/jquinn/lammps/src/lammps.cpp: In member function 'void
LAMMPS_NS::LAMMPS::init_pkg_lists()':
/home/jquinn/lammps/src/lammps.cpp:895:13: note: variable tracking size limit exceeded with
'-fvar-tracking-assignments', retrying without
  895 | void _noopt LAMMPS::init_pkg_lists()
      |             ^~~~~
make[1]: *** [CMakeFiles/Makefile2:996: CMakeFiles/lammps.dir/all] Error 2
make: *** [Makefile:150: all] Error 2
jquinn@DESKTOP-D7PCTBN:~/lammps/build_4$
```

Tried to work through the problems raised when Building LAMMPS

My C++ skills are still not great as i haven't had time to develop much lately

Emailed Mehran Today my problem

+ about a potential meeting about this problem specifically

I would have met / spoke with him earlier but I didn't want to waste his time so I wanted to wait until I had a specific problem to work through with him

Got some Files to show Mehran for Help / meeting

"Fluidmembrane" Files
LJ Cut Files
Frankenstien Files
LAMMPS Error Codes

Today Worked a little (~ 30 Min) on geometry file

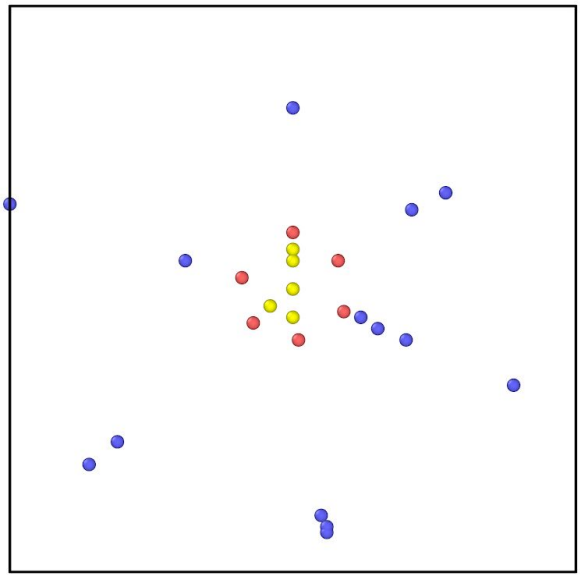
Currently have a bug

Step of range function used in placing particles is too large

The range function steps across the 2 radial direction with a far too wide step, meaning that it only will place a particle every radian

This is due to the range function only being able to step by integers

Might need to find a Python Module with a more exact calculation for range
Or Write another custom function to do the same



Other "To-Do's" for Geometry File

I think they use a elliposid atom style for some of their particles

\+ More once bug is figured out probably

Email LAMMPS Mailing List with Sameish question ot mehran

MEMbrane Stablity

1 tyro to use Scott Diamond paper files

Email the Tan Author and CC Scott diamond

Ask how exactly they used LAMMPS
As library or exe?

More?

Meet wth mehran when I can but

Until then work on Diamond Paper

Look at LAMMPS files to see if they have a Potential field guide

If not see if they have patch notes pertaining to potential compatibility