User guide for CFD–DEM solver lammpsFoam

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1 Introduction

Here is the brief introduction of demFoam, a toolbox of CFD–DEM simulation:

"demFoam" is the name of this toolbox.

"lammpsFoam" is an open source CFD–DEM solver combining the LAMMPS and openFoam.

"LAMMPS" is an open source molecular dynamics code that perform DEM simulations.

"OpenFOAM" is an open source toolbox for CFD simulations.

The structure of the demFoam is like this:

```
demFoam
|−−−−Allwclean.sh
|−−−−Allwmake.sh
|−−−−cases/
|−−−−documentation/
|−−−−interfaceToLammps/
|−−−−lammpsFoam/
|−−−−readme/
```

"Allwclean.sh" and "Allwmake.sh" are written to help with the compilation of lammpsFoam, the CFD–DEM solver in demFoam. "Allwmake.sh" will help you install lammpsFoam while "Allclean.sh" will uninstall lammpsFoam. Note that the source file of LAMMPS is not included in demFoam. We highly recommend you use lammps-1Feb14, a version released on February 2014.

All numerical cases are placed in "demFoam/cases/", including verification cases and validations cases.

Some documents are in "demFoam/documentation/", with a basic user manual (userManual.tex).

"demFoam/interfaceToLammps/" and "demFoam/lammpsFoam/" are folders containing the source code of lammpsFoam. To compile lammpsFoam, the files of "demFoam/interfaceToLammps/" should be copied to "LAMMPS-(some version)/src". Allwclean.sh are Allwmake.sh written to help with the compilation of lammpsFoam, the CFD–DEM solver

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2   How to install lammpsFoam on your linux machine?

Although Allwmake.sh can automatically help you with the installation of lammpsFoam, it is necessary to demonstrate individual steps in the compilation.

2.1   Environment for lammpsFoam

The CFD-DEM solver lammpsFoam would be successfully installed on a machine with OpenFOAM and LAMMPS. Here are the steps to compile it on your linux machine:

1. Install OpenFOAM on your machine, the up-to-date lammpsFoam is supported for Open-FOAM 2.3.0, 2.3.x, and 2.4.0.

2. Copy all the files in "InterfaceToLammps" folder to "lammps-1Feb14/src", or create a soft link of the files.

3. Copy all the files in "InterfaceToLammps/MAKE" folder to "lammps-1Feb14/src/MAKE", or create a soft link of the files.

4. Change to the "lammps-1Feb14/src" folder. Use command "make yes-granular" to install the granular package of LAMMPS. Add "kspace", "manybody", "molecule", "fld", "rigid", "misc" as well in a similar way.

5. Go back to the "lammps-1Feb14/src" folder. Use command "make shanghailinux" to generate an executable file named "lmp_shanghailinux" in this folder. It may take a while.

6. Stay at "lammps-1Feb14/src" folder. Use command "make makeshlib" to generate a new "Makefile.shlib" file.

7. Stay at "lammps-1Feb14/src" folder. Use command "make -f Makefile.shlib shanghailinux" to compile LAMMPS to a dynamic library. After this step, you will see a file named "liblammps_shanghailinux.so".

8. Change to "$FOAM_USER_LIBBIN" and make a soft link of "liblammps_shanghailinux.so" in this folder. "liblammps_shanghailinux.so" is the file generated in the previous step.

9. Change to "LammpsFoam" folder. Use command "wmake libso dragModels" to compile the drag models. Use command "wmake libso chPressureGrad" to compile the pressure gradient for channel flow. Use command "wmake libso lammpsFoamTurbulenceModels" to compile the turbulent models for lammpsFoam.

10. 10.Change to "lammpsFoam/Make" folder. Choose the file named "options-*-openmpi" (* is the name of operating system called OS thereafter) according to your own OS and rename it as the file named "options". (For example, if your OS is ubuntu, choose the file named "options-ubuntu-openmpi" and rename it as "options") Then, you should modify the first line which represents the path of lammps/src directory in the "options" file. Default path is "LAMMPS_DIR = ../lammps-1Feb14/src", you should replace "../lammps-1Feb14" with the path where you installed your own lammps package and the correct version name of your lammps package.

11. Stay at the same directory. Use command "wmake" to compile the lammpsFoam solver.

To check if your lammpsFoam is succesfully compiled, you can:

1. Change to the "cases/auto-testing/test-cases/xiaocase3/" folder.

2. Execute "./Allrun.sh" in the command line to see the result.

3   Cases and supporting publications

There are lot of publications using lammpsFoam [**?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**, **?**]:
  Several cases from the publications are added in "demfoam/cases/auto-testing/test-cases":

1. "xiaocase1" is the 1st case in H. Xiao et al.'s paper [**?**].

2. "xiaocase3" is the 3rd case in H. Xiao et al.'s paper [**?**].

3. "expMuller09" is the case in R. Sun et al.'s paper [**?**, **?**].