Installation of LAMMPS-27Mar12 - 28May12 on OS X 10.7 (Lion)

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LAMMPS is a software for molecular (and particles) dynamics.
It can be installed on Mac OS X with several steps.
On multi-cores macbook, lammps is installed with fftw 3.x and open mpi.
This document corresponds to lammps-27May12 and lammps-28May12.

LAMMPS Molecular Dynamics Simulator
http://lammps.sandia.gov/

Remark: new package USER-COLVARS is added on lammps-27May12.
Remark: built without CUDA package.
Remark: OS X 10.6 or later is necessary for GPU/OpenCL package.

(1) OS X 10.7.x (lion) is used with MacBook Core2Duo (late 2009).
(2) Xcode 4.x for OS X 10.7.x is installed.
  # Xcode is Apple's development tool for OS X and can be obtained from http://developer.apple.com/ (You need an account for this site.)
remark: if you use xcode 4.3 or later, you need to install command line tools for it.
(3) downloading gfortran from http://hpc.sf.net : gfortran-lion.tar.gz for os x 10.7.x
instruction:
(A) $ gunzip gfortran-lion.tar.gz
(B) $ sudo tar -xf gfortrn-lion.tar -C /
(3') you can also obtain gfortran from: Tools - R for Mac OS X - developer's page - GNU Fortan for Xcode
(4.1) installation of OpenMPI
downloading OpenMPI from http://www.open-mpi.org/software/ompi/v1.4/
extracting tar file (double clicking tar.gz file) and:
$ ./configure
$ make all
$ make check
$ sudo make install
(4.2) installation of FFTW
we employ FFTW version 3.x # 29 February 2012
http://www.fftw.org/download.html
extracting tar file (double clicking tar.gz file) and:
$ ./configure
$ make all
$ make check
$ sudo make install
(5) installing OpenKIM (Open Knowledge base Interatomic Model)
download KIM API from https://openkim.org/kim_api
  #We employed version 1.0.1 or later.
Extract the file and On Terminal
$ export KIM_DIR=”the path to openkim” # ending with “/”
# example: KIM_DIR = /Users/foo/openkim-api-v1.0.1/
$ cd $KIM_DIM
$ make

(6) Downloading Lammps
the latest version is obtained from below:
http://lammps.sandia.gov/download.html#tar
old versions are obtained from below:
http://lammps.sandia.gov/tars/

(7) building LAMMPS
Remark: in Makefile, tab is used for spacing.
(A) build libraries: awpmd, atc, meam, poem, reax, gpu, colvars.
at awpmd:
modification of Makefile.lammps:
user-awpmd_SYSINC =
user-awpmd_SYSLIB = -framework vecLib # use apple lapack and blas
user-awpmd_SYSPATH =

```
$ make -f Makefile.openmpi
```

at atc:
modification of Matrix.cpp:

```
#include "DenseMatrix.h"
#include "Solver.h"
#include "SparseMatrix.h"          // added on 28 september 2011
#include "DiagonalMatrix.h"        // added on 28 september 2011
```

modification of Makefile.lammps:

```
user-awpmd_SYSINC =
user-awpmd_SYSLIB = -framework vecLib # use apple lapack and blas
user-awpmd_SYSPATH =
```

```
$ make -f Makefile.g++
```

at meam:
modification of Makefile.lammps:

```
meam_SYSINC =
meam_SYSLIB = -lgfortran          # for gfortran
meam_SYSPATH =
```

```
$ make -f Makefile.gfortran
```

at poems:

```
$ make -f Makefile.g++
```

at reax:
modification of Makefile.lammps:

```
meam_SYSINC =
meam_SYSLIB = -lgfortran          # for gfortran
meam_SYSPATH =
```

```
$ make -f Makefile.gfortran
```

at gpu (OpenCL)
modification of Makefile.lammps:

```
gpu_SYSINC =
gpu_SYSLIB = -framework OpenCL    # use apple opencl framework
gpu_SYSPATH =
```

```
$ make -f Makefile.mac_opencl
```

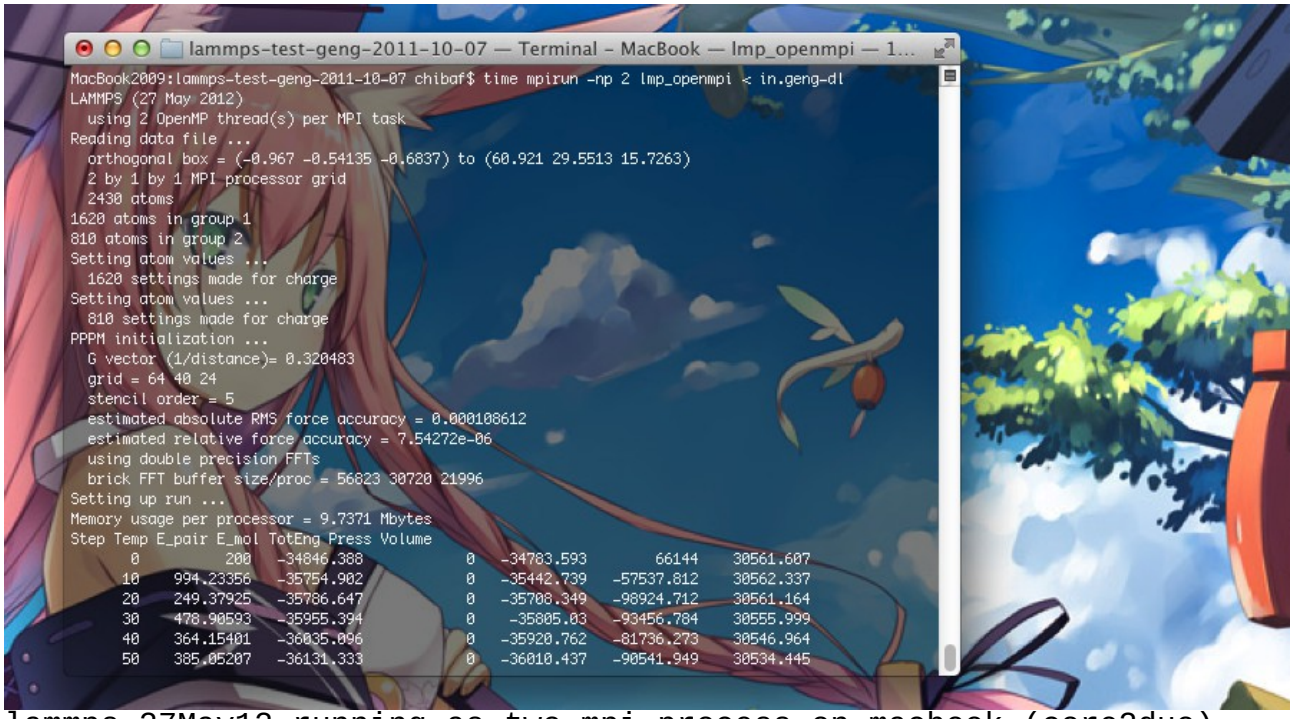
at colvars

```
$ make -f Makefile.g++

(B) at src/MAKE:
modification of Makefile.openmpi
CC =            mpic++
CCFLAGS =       -O2 \
                -funroll-loops -fstrict-aliasing -Wall -W -Wno-
uninitialized -fopenmp   # use openmp
DEPFLAGS =      -M
LINK =          mpic++
LINKFLAGS =     -O -lgfortran -framework vecLib -lgomp # for
gfortran and openmp; use apple lapack and blas
.......
.......
# FFT library, OPTIONAL
# see discussion in doc/Section_start.html#2_2 (step 6)
# can be left blank to use provided KISS FFT library
# INC = -DFFT setting, e.g. -DFFT_FFTW, FFT compiler settings
# PATH = path for FFT library
# LIB = name of FFT library

FFT_INC = -DFFT_FFTW3 # use fftw 3.x
FFT_PATH =
FFT_LIB = -lfftw3 # use fftw 3.x
(C) at KIM/
modification of Install.sh(*); on line 15
#   sed -i '4 i include ..\/..\/lib\/kim\/Makefile.lammps'
../Makefile.package.settings
# multiline form needed for BSD sed on Macs
    sed -i -e '4 i \
include ..\/..\/lib\/kim\/Makefile.lammps\
' ../Makefile.package.settings
(*)thanks to " [lammps-users] Issues installing packages on Mac" by G. Tauriello
(D) generating makefile at src directory
$ make yes-all #adding all packages
$ make no-user-cuda  #deleting CUDA package
(E)at src
build executable binary: lmp_openmpi
$ export KIM_DIR = "the path to openkim directory"
# example: KIM_DIR = /Users/foo/openkim-api-v1.0.1
$ make openmpi
(F) setting example
suppose that a directory ~/bin exists.
$ cp lmp_openmpi ~/bin/
$ export PATH=$PATH:~/bin         # use it in .bash_profile
```

(8) execution of Lammps as multi-process
command for multi process:
$ mpirun -np N lmp_openmpi < in.lammps.script
#N is a number of MPI process
#see Lammps manual for details.

command for multi threads with OpenMP:
$ mpirun -x OMP_NUM_THREADS=2 -np 2 lmp_openmpi -sf omp -in in.lammps
# two mpi process and two openmp threads per mpi process

```
MacBook2009:~ chibaf$ ps -M
USER     PID   TT   %CPU STAT PRI     STIME     UTIME COMMAND
chibaf 25330 s000    0.0 S    31T   0:00.01   0:00.01 -bash
chibaf 25344 s000    0.0 S    31T   0:00.01   0:00.01 mpirun -x OMP_NUM_THREADS=2 -np 2 lmp_openmpi
chibaf 25345 s000   45.7 R     7T   0:03.29   0:14.66 lmp_openmpi -sf omp -in in.lammps
       25345        18.1 S    23T   0:00.05   0:08.42
chibaf 25346 s000   57.3 R     4T   0:02.11   0:16.00 lmp_openmpi -sf omp -in in.lammps
       25346        20.1 S    22T   0:00.06   0:09.51
chibaf 25350 s003    0.0 S    31T   0:00.01   0:00.00 -bash
```



lammps-27May12 running as two mpi process on macbook (core2duo)
via "a big tree of black honey and a sprig of hot water" / illustration by poko [pixiv] (in japanese)

My web site:
http://math.digi2.jp/
http://math.digi2.jp/math/lammps/ : lammps