解压之后进入 ./lib/;

进入各个文件夹执行 make –f Makefile.xxxxx

Atc make –f mpic++

Awpmd make –f mpicc

Colvars make –f g++

Meam make –f gfortran

进入 src/MAKE/OPTION

Vim Makefile.intel\_cpu

修改以下参数

# intel\_cpu = USER-INTEL package with CPU optimizations, Intel MPI, MKL FFT

SHELL = /bin/sh

# ---------------------------------------------------------------------

# compiler/linker settings

# specify flags and libraries needed for your compiler

CC =            icpc

CCFLAGS =       -g -O3 -openmp -DLAMMPS\_MEMALIGN=64 -no-offload \

                -xHost -fno-alias -ansi-alias -restrict -override-limits

SHFLAGS =       -fPIC

DEPFLAGS =      -M

LINK =          icpc

LINKFLAGS =     -g -O3 -openmp -xHost

LIB =

SIZE =          size

ARCHIVE =       ar

ARFLAGS =       -rc

SHLIBFLAGS =    -shared

# ---------------------------------------------------------------------

# LAMMPS-specific settings, all OPTIONAL

# specify settings for LAMMPS features you will use

# if you change any -D setting, do full re-compile after "make clean"

# LAMMPS ifdef settings

# see possible settings in Section 2.2 (step 4) of manual

LMP\_INC =       -DLAMMPS\_GZIP -DLAMMPS\_JPEG

# MPI library

# see discussion in Section 2.2 (step 5) of manual

# MPI wrapper compiler/linker can provide this info

# can point to dummy MPI library in src/STUBS as in Makefile.serial

# use -D MPICH and OMPI settings in INC to avoid C++ lib conflicts

# INC = path for mpi.h, MPI compiler settings

# PATH = path for MPI library

# LIB = name of MPI library

MPI\_INC =       -DMPICH\_SKIP\_MPICXX -DOMPI\_SKIP\_MPICXX=1 -I/opt/mpich/include

MPI\_PATH =      -L/opt/mpich/lib

MPI\_LIB =       -lmpich -lmpl -lpthread

# FFT library

# see discussion in Section 2.2 (step 6) of manaul

# 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\_MKL -I/work/opt/intel/mkl/include/fftw

FFT\_PATH =      -L/work/opt/intel/mkl/interfaces/fftw3xf

FFT\_LIB =       -L$MKLROOT/lib/intel64/ -lmkl\_intel\_ilp64 \

                -lmkl\_intel\_thread -lmkl\_core

# JPEG and/or PNG library

# see discussion in Section 2.2 (step 7) of manual

# only needed if -DLAMMPS\_JPEG or -DLAMMPS\_PNG listed with LMP\_INC

# INC = path(s) for jpeglib.h and/or png.h

# PATH = path(s) for JPEG library and/or PNG library

# LIB = name(s) of JPEG library and/or PNG library

JPG\_INC =

JPG\_PATH =

JPG\_LIB =       -ljpeg

# ---------------------------------------------------------------------

# build rules and dependencies

# do not edit this section

include Makefile.package.settings

include Makefile.package

EXTRA\_INC = $(LMP\_INC) $(PKG\_INC) $(MPI\_INC) $(FFT\_INC) $(JPG\_INC) $(PKG\_SYSINC)

EXTRA\_PATH = $(PKG\_PATH) $(MPI\_PATH) $(FFT\_PATH) $(JPG\_PATH) $(PKG\_SYSPATH)

EXTRA\_LIB = $(PKG\_LIB) $(MPI\_LIB) $(FFT\_LIB) $(JPG\_LIB) $(PKG\_SYSLIB)

# Path to src files

vpath %.cpp ..

vpath %.h ..

# Link target

$(EXE): $(OBJ)

        $(LINK) $(LINKFLAGS) $(EXTRA\_PATH) $(OBJ) $(EXTRA\_LIB) $(LIB) -o $(EXE)

        $(SIZE) $(EXE)

# Library targets

lib:    $(OBJ)

        $(ARCHIVE) $(ARFLAGS) $(EXE) $(OBJ)

shlib:  $(OBJ)

修改完成之后 cd ../..

Make clean-all;

make yes-\*\*\*\*\*

这是lammps-9Dec14可以用的列表

Installed YES: package ASPHERE

Installed YES: package BODY

Installed YES: package CLASS2

Installed YES: package COLLOID

Installed YES: package DIPOLE

Installed YES: package FLD

Installed  NO: package GPU

Installed YES: package GRANULAR

Installed  NO: package KIM

Installed  NO: package KOKKOS

Installed YES: package KSPACE

Installed YES: package MANYBODY

Installed YES: package MC

Installed YES: package MEAM

Installed YES: package MISC

Installed YES: package MOLECULE

Installed  NO: package MPIIO

Installed YES: package OPT

Installed YES: package PERI

Installed YES: package POEMS

Installed YES: package QEQ

Installed YES: package REAX

Installed YES: package REPLICA

Installed YES: package RIGID

Installed YES: package SHOCK

Installed YES: package SNAP

Installed YES: package SRD

Installed  NO: package VORONOI

Installed YES: package XTC

Installed  NO: package USER-ATC

Installed  NO: package USER-AWPMD

Installed YES: package USER-CG-CMM

Installed YES: package USER-COLVARS

Installed  NO: package USER-CUDA

Installed YES: package USER-EFF

Installed YES: package USER-FEP

Installed YES: package USER-INTEL

Installed  NO: package USER-LB

Installed YES: package USER-MISC

Installed YES: package USER-MOLFILE

Installed YES: package USER-OMP

Installed YES: package USER-PHONON

Installed YES: package USER-QMMM

Installed YES: package USER-REAXC

Installed YES: package USER-SPH

最后执行 make intel\_cpu

lammps-3Feb16可用列表

Installed YES: package ASPHERE

Installed YES: package BODY

Installed YES: package CLASS2

Installed YES: package COLLOID

Installed YES: package COMPRESS

Installed YES: package CORESHELL

Installed YES: package DIPOLE

Installed YES: package FLD

Installed  NO: package GPU

Installed YES: package GRANULAR

Installed  NO: package KIM

Installed  NO: package KOKKOS

Installed YES: package KSPACE

Installed YES: package MANYBODY

Installed YES: package MC

Installed YES: package MEAM

Installed YES: package MISC

Installed YES: package MOLECULE

Installed  NO: package MPIIO

Installed YES: package OPT

Installed YES: package PERI

Installed YES: package POEMS

Installed  NO: package PYTHON

Installed YES: package QEQ

Installed YES: package REAX

Installed YES: package REPLICA

Installed YES: package RIGID

Installed YES: package SHOCK

Installed YES: package SNAP

Installed YES: package SRD

Installed  NO: package VORONOI

Installed YES: package XTC

Installed  NO: package USER-ATC

Installed  NO: package USER-AWPMD

Installed YES: package USER-CG-CMM

Installed YES: package USER-COLVARS

Installed  NO: package USER-CUDA

Installed YES: package USER-DIFFRACTION

Installed YES: package USER-DPD

Installed YES: package USER-DRUDE

Installed YES: package USER-EFF

Installed YES: package USER-FEP

Installed  NO: package USER-H5MD

Installed YES: package USER-INTEL

Installed  NO: package USER-LB

Installed YES: package USER-MGPT

Installed YES: package USER-MISC

Installed YES: package USER-MOLFILE

Installed YES: package USER-OMP

Installed YES: package USER-PHONON

Installed YES: package USER-QMMM

Installed YES: package USER-QTB

Installed  NO: package USER-QUIP

Installed YES: package USER-REAXC

Installed  NO: package USER-SMD

Installed YES: package USER-SMTBQ

Installed YES: package USER-SPH

Installed YES: package USER-TALLY