Compiling LAMMPS

because sometimes you just have to

Chris MacDermaid
26-March-2014

First things first

- If you're using the lammps-ictp virtual machine:
  - Increase the VM processor-count to 4
  - you'll need to install fftw, openmpi and libjpeg
    `su -c 'yum install fftw-static openmpi-devel libjpeg-turbo-static'`
  - LAMMPS source: `~ictp/Downloads/lammps-vanilla`
- If you're using your own machine, you'll need to download LAMMPS, and if you want to compile with fftw/openmpi enabled binaries, you'll need to install those packages as well. You'll probably need to install gcc/g++ as well.

LAMMPS Directory Structure

```
ictp@localhost~/Downloads/lammps-vanilla
├── bench
├── doc
├── examples
├── lib
│   └── reax
├── potentials
├── python
├── regress
├── src
│   ├── MAKE
│   ├── MOLECULE
│   ├── USER-OMP
└── tools
```

Top-level Make

```
ictp@localhost ~/Downloads/lammps-vanilla/src $ make

make clean-all                  delete all object files
make clean-machine              delete object files for one machine
make purge                      purge obsolete copies of package sources
make tar                        create lmp_src.tar.gz of src dir and packages
make makelib                    create Makefile.lib for static library build
make makeshlib                  create Makefile.shlib for shared library build
make makelist                   create Makefile.list used by old makes
make -f Makefile.lib machine    build LAMMPS as static library for machine
make -f Makefile.shlib machine  build LAMMPS as shared library for machine
make -f Makefile.list machine   build LAMMPS from explicit list of files
make stubs                      build dummy MPI library in STUBS
make install-python             install LAMMPS wrapper in Python

. . .
```

Package Installation

make yes-user-omp
make yes-kspace

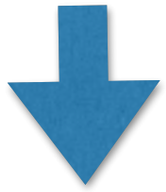
```
Standard packages: asphere body class2 colloid dipole fld gpu granular kim kspace manybody mc
meam misc molecule mpiio opt peri poems reax replica rigid shock srd voronoi xtc

User-contributed packages: user-atc user-awpmd user-cg-cmm user-colvars user-cuda user-eff
user-lb user-misc user-omp user-molfile user-phonon user-reaxc user-sph

make package                list available packages
make package-status (ps)    status of all packages
make yes-package            install a single package in src dir
make no-package             remove a single package from src dir
make yes-all                install all packages in src dir
make no-all                 remove all packages from src dir
make yes-standard           install all standard packages
make no-standard            remove all standard packages
make yes-user               install all user packages
make no-user                remove all user packages
make no-lib                 remove all packages with external libs
```

machine makefiles

Machine /src/MAKE/Makefile.machine



```
src> make -j4 serial
```

```
# altix = SGI Altix, Intel icc, MPI, FFTs from SGI SCSL library
# bgl = LLNL Blue Gene Light machine, xlC, native MPI, FFTW
# chama - Intel sandybridge with dual socket/eight core nodes, mpic++, openmpi, no FFTW
# cygwin = Windows Cygwin, mpicxx, MPICH, FFTW
# encanto = NM cluster with dual quad-core Xeons, mpicxx, native MPI, FFTW
# fink = Mac OS-X w/ fink libraries, c++, no MPI, FFTW 2.1.5
# g++ = RedHat Linux box, g++4, MPICH2, FFTW
# g++3 = RedHat Linux box, g++ (v3), MPICH2, FFTW
. . .
# openmpi = Fedora Core 6, mpic++, OpenMPI-1.1, FFTW2
# serial =  RedHat Linux box, g++4, no MPI, no FFTs
. . .
# xe6 = Cray XE6, Cray CC, native MPI, FFTW
# xt3 = PSC BigBen Cray XT3, CC, native MPI, FFTW
# xt5 = Cray XT5, Cray CC, native MPI, FFTW
```

The naive first attempt:

- `make yes-all`
  `make -j4 machine`

- What you've just done: Installed **ALL** packages, some requiring libraries that need to be compiled before building LAMMPS.

- What can I do? Install only the packages you need, and compile the necessary libraries under *lib* before building.

Serial

- The serial version uses mpi stubs (dummy MPI library) and kiss-fft (included)

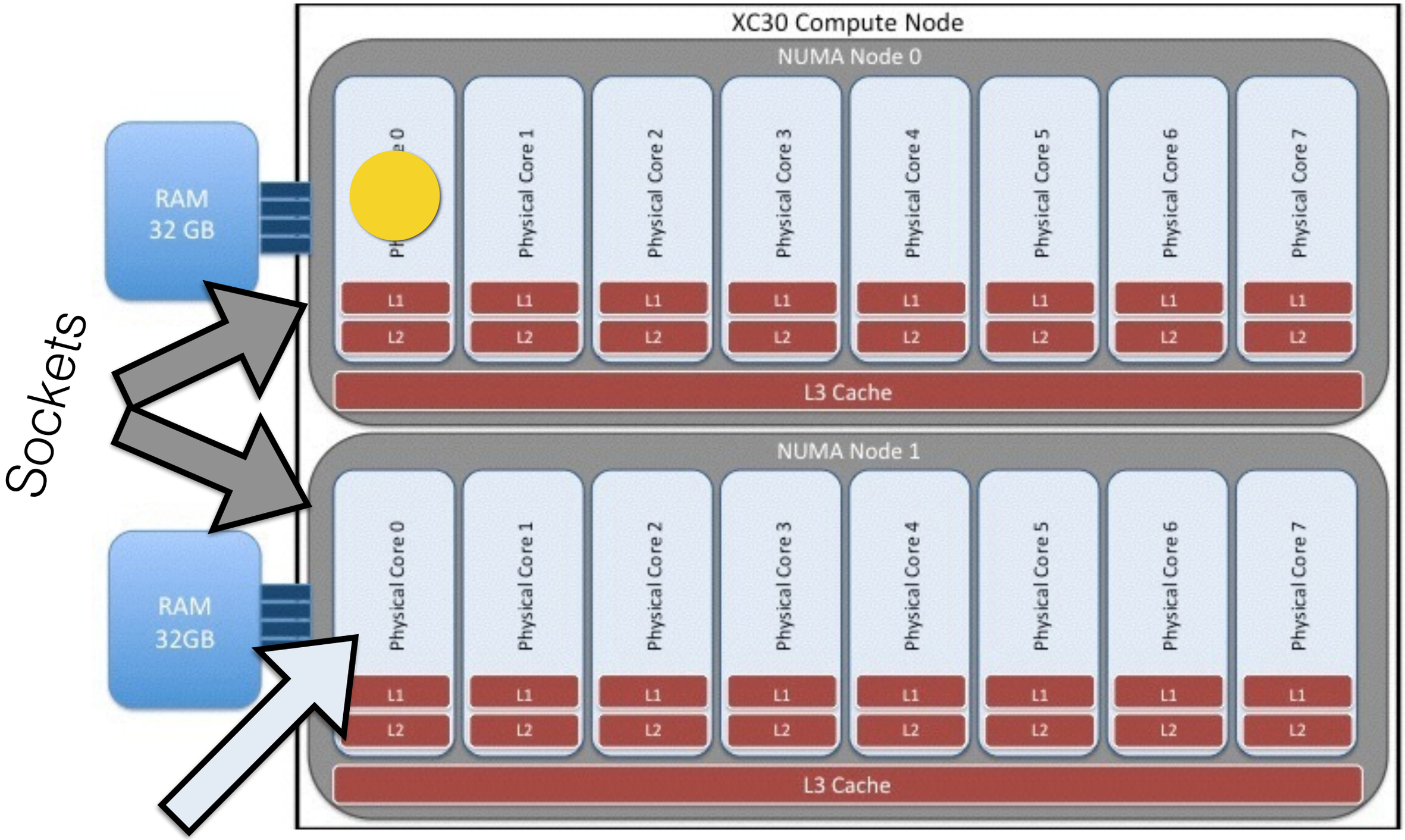
- You'll need to compile the mpi stubs first
  src> `make stubs`

- src> `make -j4 serial`

- run lj.melt benchmark
  bench> `../src/lmp_serial < in.lj`

- Note the loop time

../src/lmp_serial < in.lj



Core

1 task - 1 thread

Cray XC30 Sandybridge based compute node. 2x8-core.

Anatomy of Makefile.serial

```
# serial = RedHat Linux box, g++4, no MPI, no FFTs

SHELL = /bin/sh

# ------------------------------------------------------------------------
# compiler/linker settings
# specify flags and libraries needed for your compiler

CC =            g++
CCFLAGS =       -O
SHFLAGS =       -fPIC
DEPFLAGS =      -M

LINK =          g++
LINKFLAGS =     -O
LIB =
SIZE =          size

ARCHIVE =       ar
ARFLAGS =       -rc
SHLIBFLAGS =    -shared
```

Description

- src/MAKE/Makefile.serial

Anatomy of Makefile.serial

```
# ---------------------------------------------------------------------
# LAMMPS-specific settings
# specify settings for LAMMPS features you will use
# if you change any -D setting, do full re-compile after "make clean"

# LAMMPS ifdef settings, OPTIONAL
# see possible settings in doc/Section_start.html#2_2 (step 4)

LMP_INC =       -DLAMMPS_GZIP

# MPI library, REQUIRED
# see discussion in doc/Section_start.html#2_2 (step 5)
# can point to dummy MPI library in src/STUBS as in Makefile.serial
# INC = path for mpi.h, MPI compiler settings
# PATH = path for MPI library
# LIB = name of MPI library

MPI_INC =       -I../STUBS
MPI_PATH =      -L../STUBS
MPI_LIB =       -lmpi_stubs
```

Preprocessor Defines

MPI

- src/MAKE/Makefile.serial

Anatomy of Makefile.serial

```
# 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

# LIB = name of FFT library

FFT_INC =
FFT_PATH =
FFT_LIB =

# JPEG and/or PNG library, OPTIONAL
# see discussion in doc/Section_start.html#2_2 (step 7)
# 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 =
```

FFTs

- src/MAKE/Makefile.serial

Image Processing

Serial: Optimized

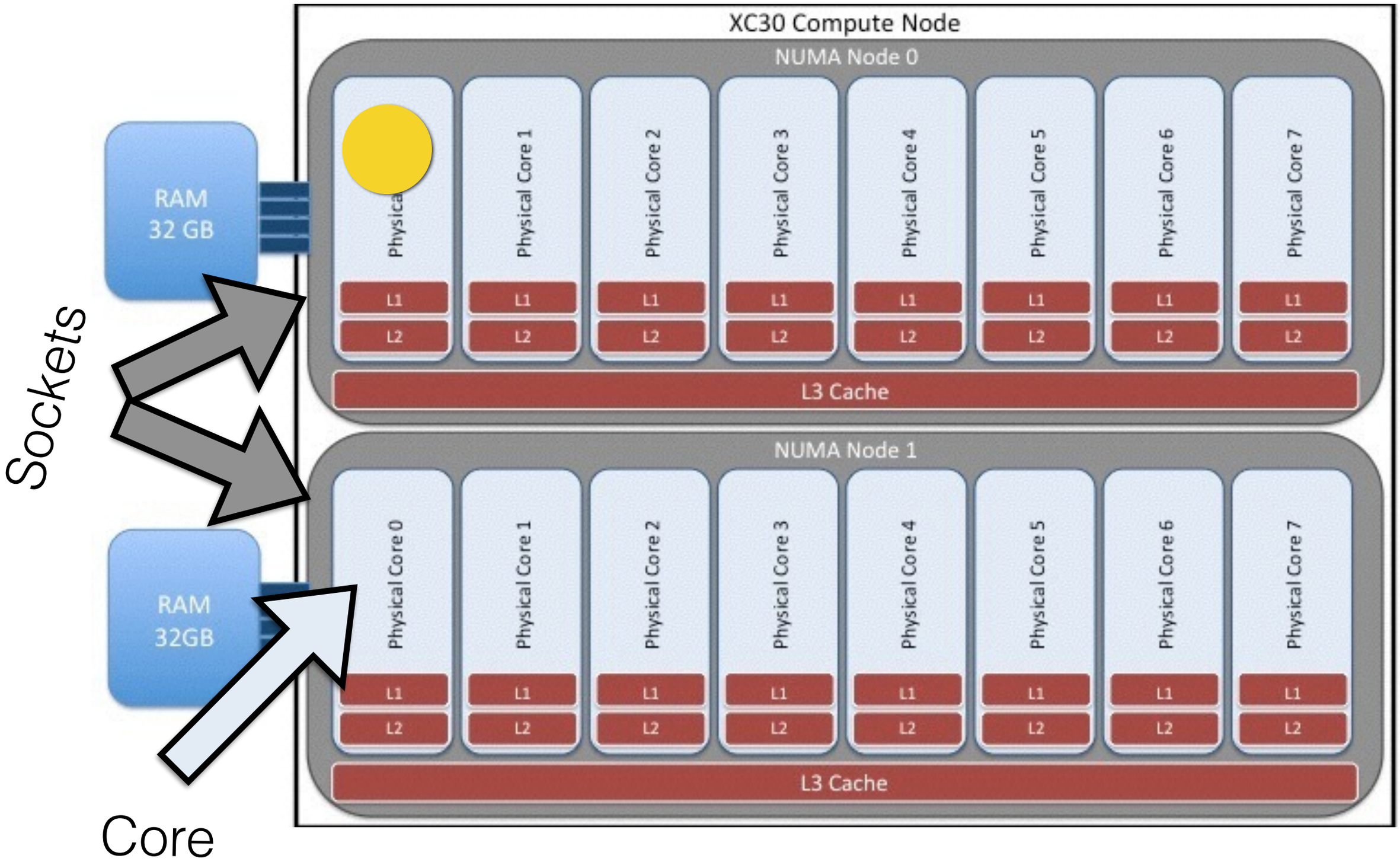
- edit src/MAKE/Makefile.serial

- Adjust compiler flags to include additional optimizations:
  `CCFLAGS =  -O2 -funroll-loops -fno-exceptions -fno-rtti`

- Recompile serial binary
  src> `make clean-serial && make -j4 serial`

- Rerun in.lj benchmark
  bench> `../src/lmp_serial < in.lj`

../src/lmp_serial < in.lj



1 task - 1 thread

External Libraries

- To write out JPEG and PNG format files, you must build LAMMPS with support for the corresponding JPEG or PNG library. Note you must hame the libjpeg/libpng library installed. To convert images into movies, LAMMPS has to be compiled with the -DLAMMPS_FFMPEG flag.

```
LMP_INC =    -DLAMMPS_GZIP -DLAMMPS_JPEG

. . .
# JPEG and/or PNG library, OPTIONAL
# see discussion in doc/Section_start.html#2_2 (step 7)
# 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
```

Packaged Libraries

- If you want to include a packaged library, you **MUST** compile that library first before compiling LAMMPS.
- lib/reax> `make -f Makefile.gfortran`
- src> `make yes-reax`
- src> `make -j4 serial`

Packaged Libraries

- In each library folder, you'll find a "`Makefile.lammps`" file which defines the additional flags required by the compiler and linker. LAMMPS automatically includes this file when you install the corresponding package.

- examine the "`src/Makefile.package`" and "`src/Makefile.package.settings`" files. Examine them after you've added or removed the reax package, for example.

Parallel: OpenMP

- Axel has implemented openmp parallelism (share everything) into LAMMPS. It's available as the 'user-omp' package.
  - a) Make a new low-level makefile by copying Makefile.serial to Makefile.omp (cp Makefile.serial Makefile.omp)
  - b) Change your compiler and linker flags to include openmp (edit src/MAKE/Makefile.omp). Change the comment at the top to reflect your new makefile.

```
#omp = Fedora20, g++4.8, MPI-stubs, KISS-FFT
CC =    g++ -fopenmp
LINK =  g++ -fopenmp
```

- c) Install the openmp package

  src> `make yes-user-omp`

- src> `make -j4 omp`

Running with OpenMP

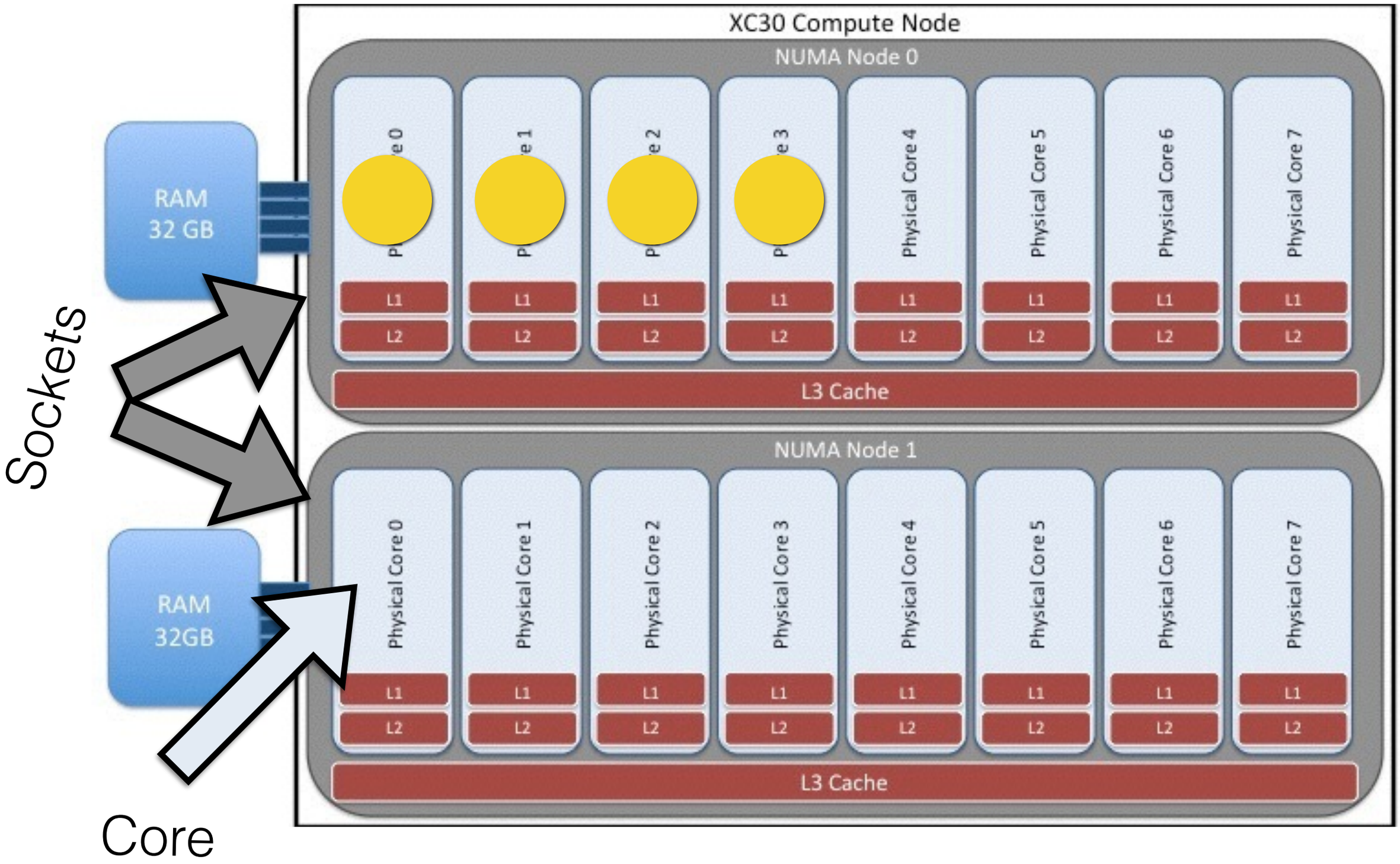
- To use your OpenMP enabled LAMMPS binary, do the following:

- To run on N processors:
  `OMP_NUM_THREADS=N lmp_omp -sf omp < in.file`

- Try running the melt example with different numbers of processors

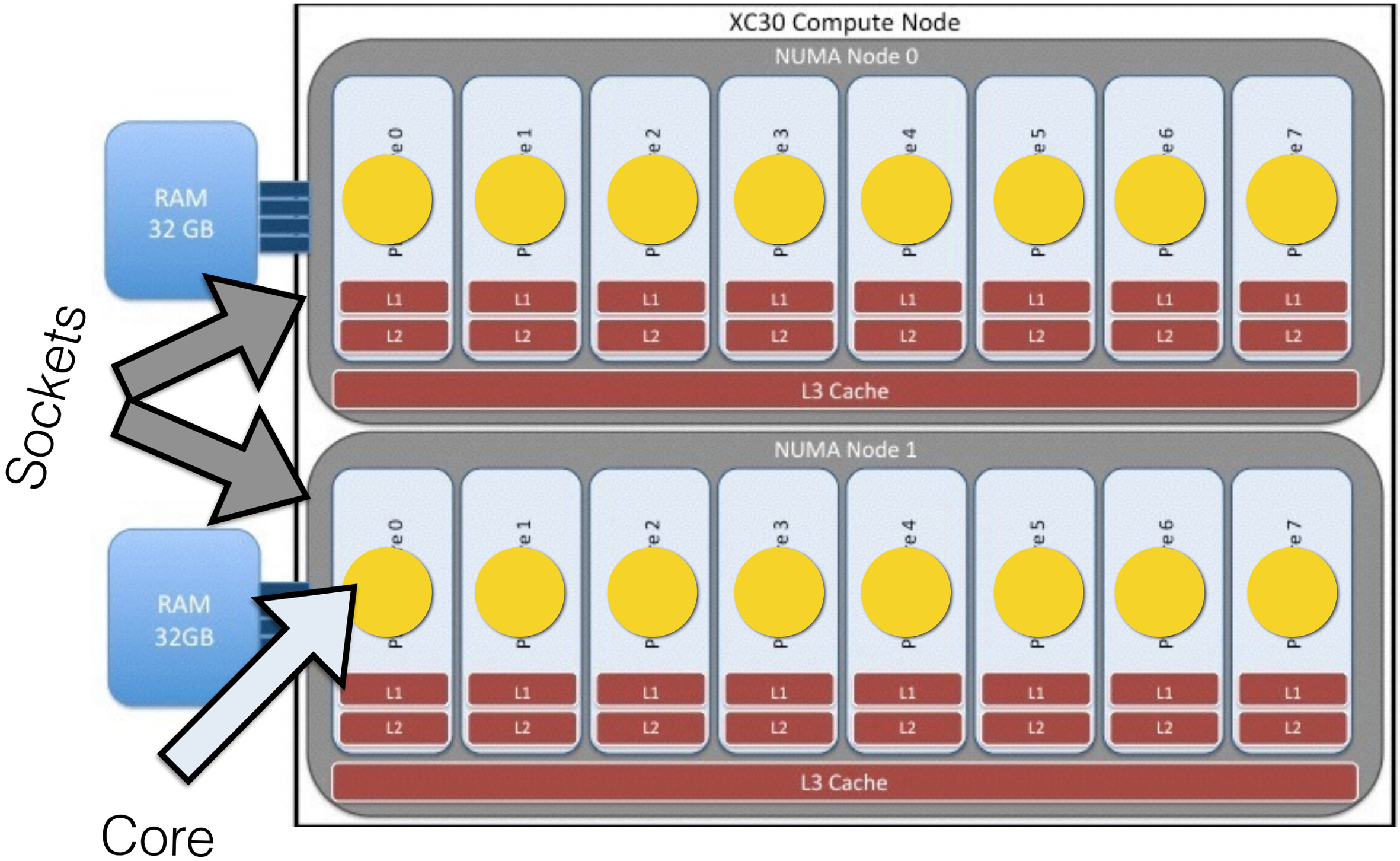
  bench> `OMP_NUM_THREADS=2 ../src/lmp_omp -sf omp < in.lj`
  bench> `OMP_NUM_THREADS=4 ../src/lmp_omp -sf omp < in.lj`

OMP_NUM_THREADS=4 ../src/lmp_omp -sf omp



1 task - 4 threads

OMP_NUM_THREADS=16 ../src/lmp_omp -sf omp



1 task - 16 threads

Biological Systems

- If you want to simulate biological systems you'll need a few additional packages: rigid (for fix shake), molecule and kspace:

- src> `make yes-molecule yes-kspace yes-rigid`

- src> make clean-omp && make -j4 omp

- bench> `OMP_NUM_THREADS=4 ../src/lmp_omp -sf omp < in.lj`
  bench> `OMP_NUM_THREADS=4 ../src/lmp_omp -sf omp < in.rhodo`

FFTW3

- Rather than use the built-in kiss-fftw library, most prefer to use the FFTW3 library. In the case of our VM, it's as easy as specifying a preprocessor directive and the library:

```
# 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 -DFFT_SINGLE
FFT_PATH =
FFT_LIB =       -lfftw3f
```

Makefile.omp

FFTW3

- Edit src/Make/Makefile.omp to include fftw3
- src> make clean-omp && make -j4 omp
- bench> `OMP_NUM_THREADS=4 ../src/lmp_omp -sf omp < in.lj`
  bench> `OMP_NUM_THREADS=4 ../src/lmp_omp -sf omp < in.rhodo`
- **Compare the loop times and FFT times, what do you notice?**

Parallel:OpenMPI

- LAMMPS' primary inter-process communication method is openMPI (share nothing). If you want to run in parallel across multiple machines, you must use openMPI.

```
CC =               mpic++
. . .
LINK =             mpic++

# MPI library, REQUIRED
# see discussion in doc/Section_start.html#2_2 (step 5)
. . .

MPI_INC =
MPI_PATH =
MPI_LIB = -lmpi
```

```
> mpicc --showme
gcc -I/usr/include/openmpi-x86_64 -pthread -m64 -L/usr/lib64/openmpi/lib -lmpi
```

Parallel:OpenMPI

- edit src/MAKE/Makefile.openmpi
  Add support for fftw3f

- Load openmpi environment variables
  `module load mpi/openmpi`

- src> `make no-user-omp`
  src> `make -j4 openmpi`

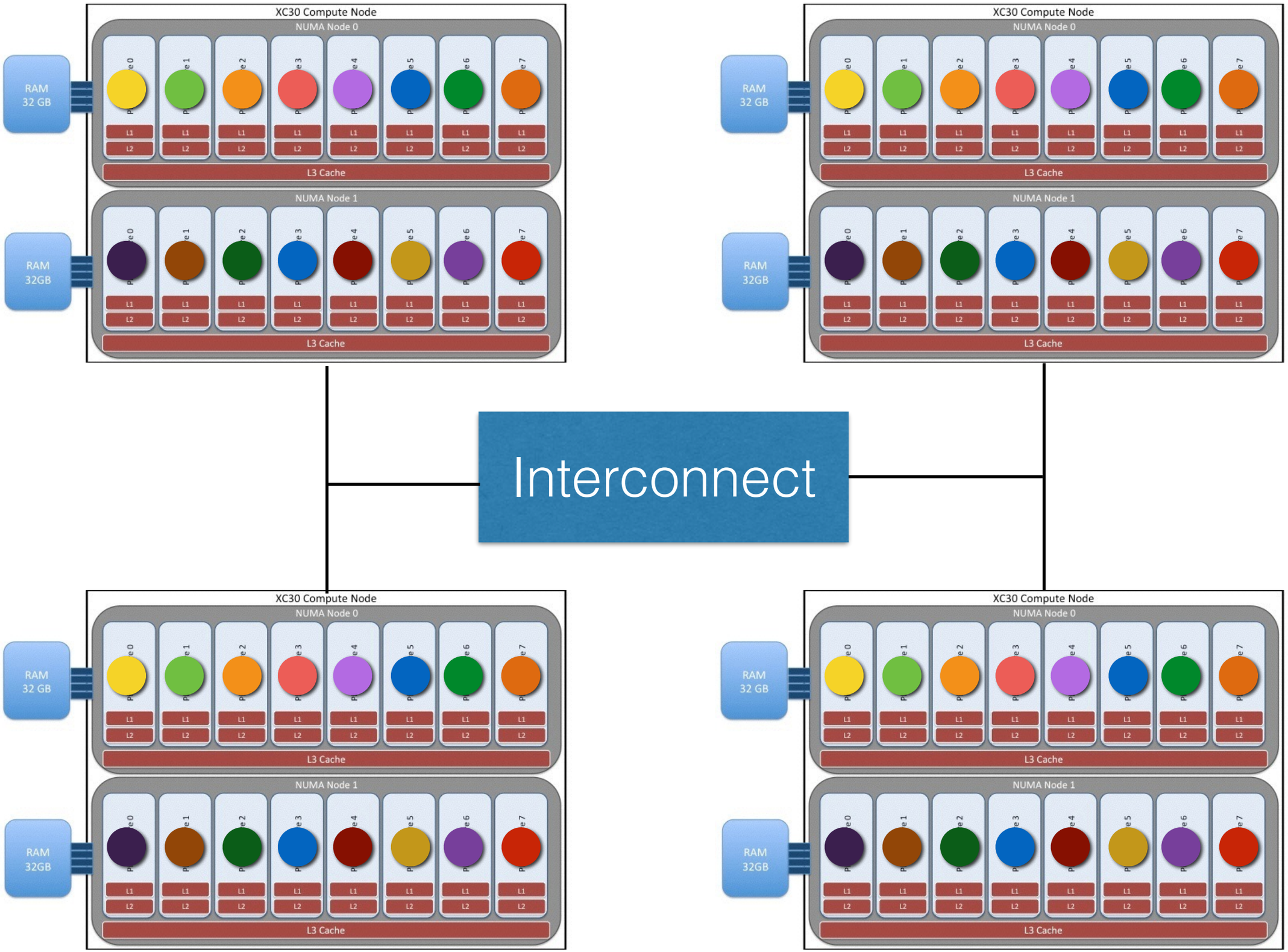
- To run on N processors:
  `mpiexec -np N lmp_openmpi < in.file`

- Try running the melt example with different numbers of processors
  bench> `mpiexec -np 2 ../src/lmp_openmpi < in.rhodo`
  bench> `mpiexec -np 4 ../src/lmp_openmpi < in.rhodo`

mpiexec -np 16 ../src/lmp_openmpi

Core 8 MPI taks per socket = 16 MPI Tasks per node

mpiexec -np 64 ../src/lmp_openmpi



Parallel: OpenMP-OpenMPI Hybrid

- You can run LAMMPS as an OpenMP-OpenMPI hybrid, where each MPI process controls a specified number of OpenMP threads. Construction of a Makefile is straightforward:

  - a) Make a new low-level makefile by copying Makefile.openmpi to Makefile.openmpi-omp (cp Makefile.omp Makefile.openmpi-omp)

  - b) Change your compiler and linker flags to include openmp (edit src/MAKE/Makefile.openmpi-omp). Change the comment at the top to reflect your new makefile.

```
#openmpi-omp = Fedora20, g++4.8, OpenMPI-1.7.3, FFTW3
CC =    mpic++ -fopenmp
LINK =  mpic++ -fopenmp
```

  - c) Install the openmp package

    src> `make yes-user-omp`

- src> `make -j4 openmpi-omp`

Running with OpenMP-OpenMPI Hybrid

- To use your OpenMPI-OpenMP enabled LAMMPS binary, do the following:

- To run N MPI tasks with M OpenMP threads:
  `OMP_NUM_THREADS=M mpiexec -np N lmp_openmpi-omp -sf omp < in.file`

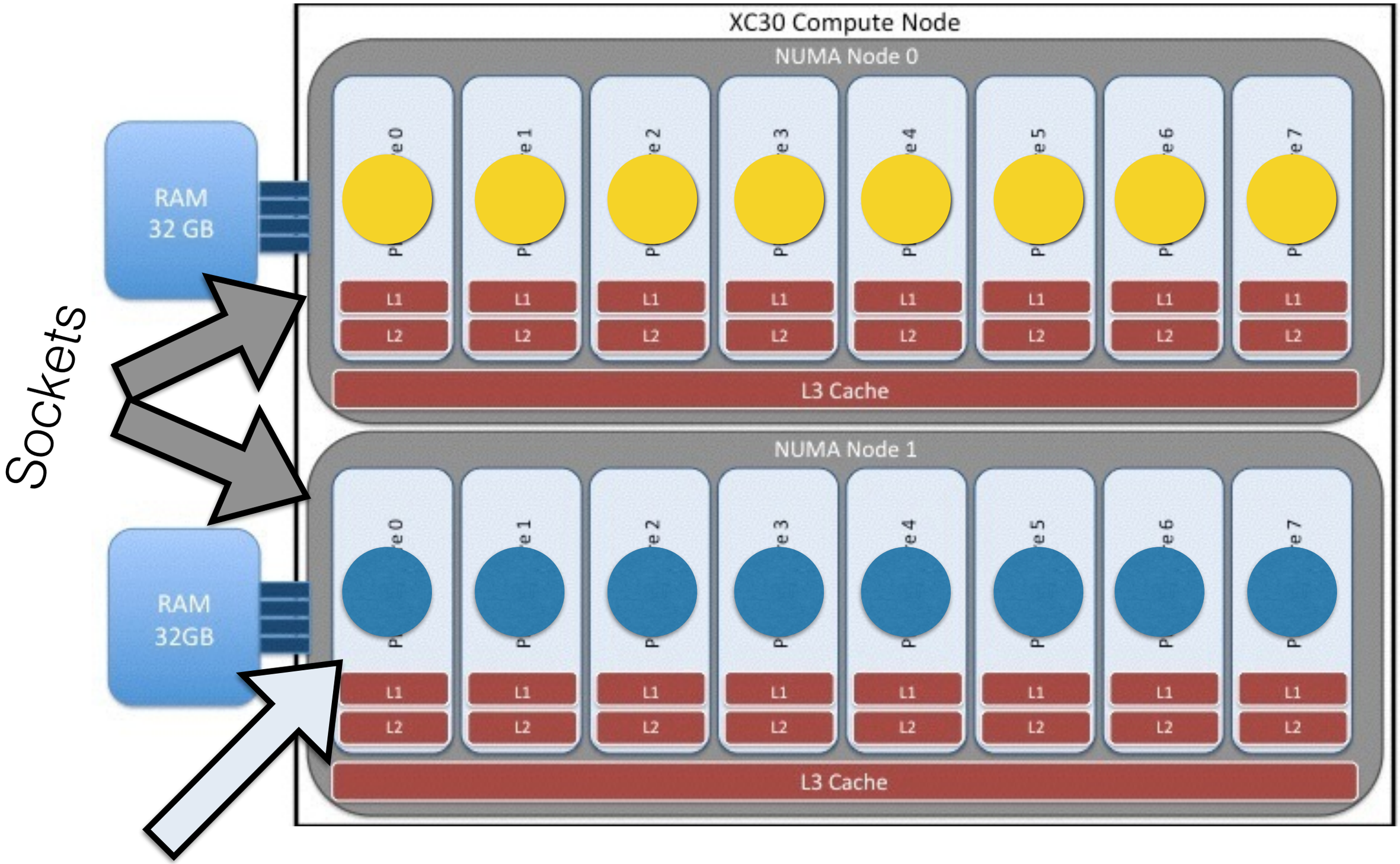
- Try running the melt and rhodo examples with different combinations of MPI tasks and omp threads

  bench> `OMP_NUM_THREADS=1 mpiexec -np 4../src/lmp_openmpi-omp -sf omp < in.lj`

  bench> `OMP_NUM_THREADS=2 mpiexec -np 2../src/lmp_openmpi-omp -sf omp < in.lj`

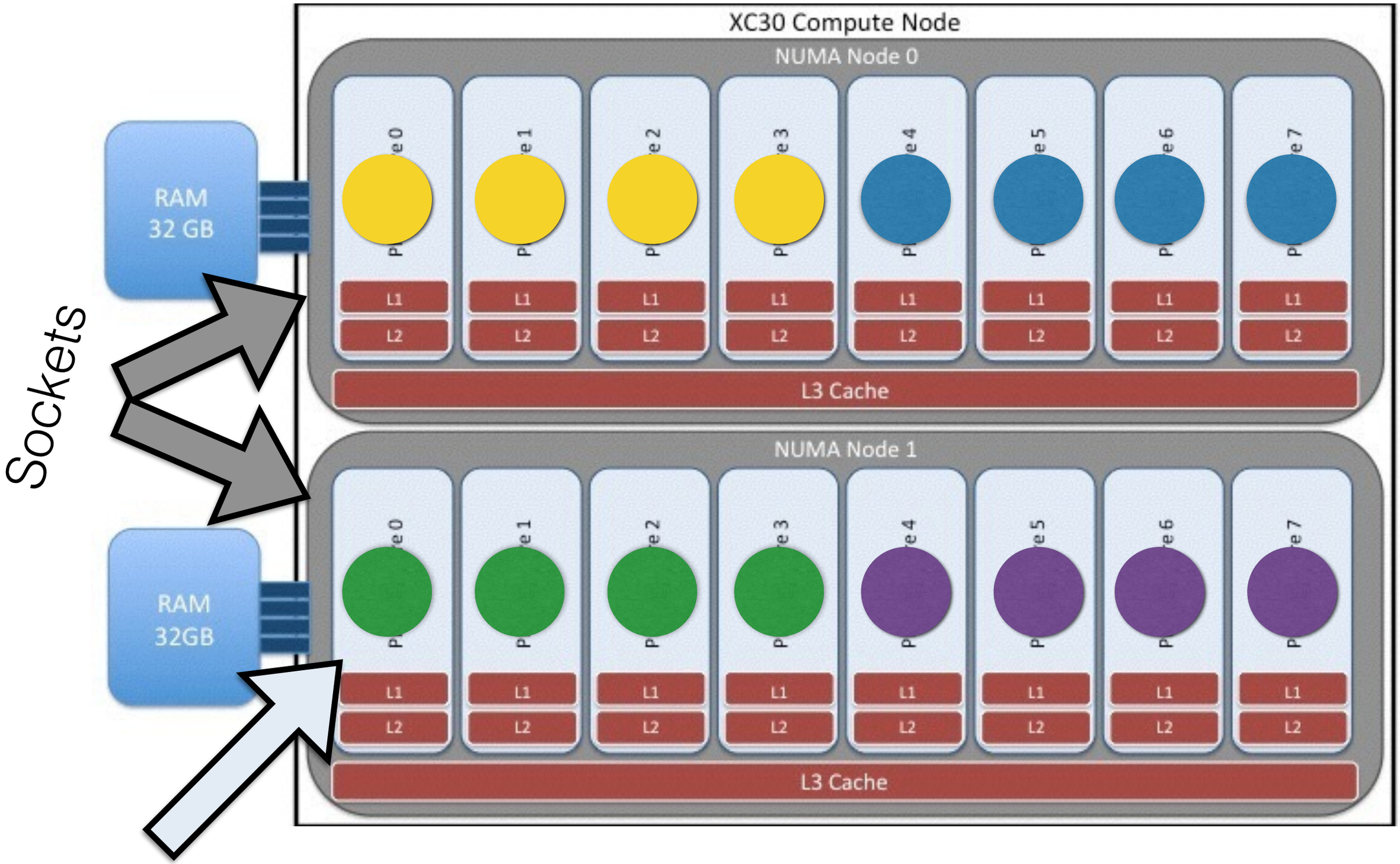
  bench> `OMP_NUM_THREADS=4 mpiexec -np 1../src/lmp_openmpi-omp -sf omp < in.lj`

```
OMP_NUM_THREADS=8 mpiexec -np 2 ../src/lmp_openmpi-omp -sf omp
```



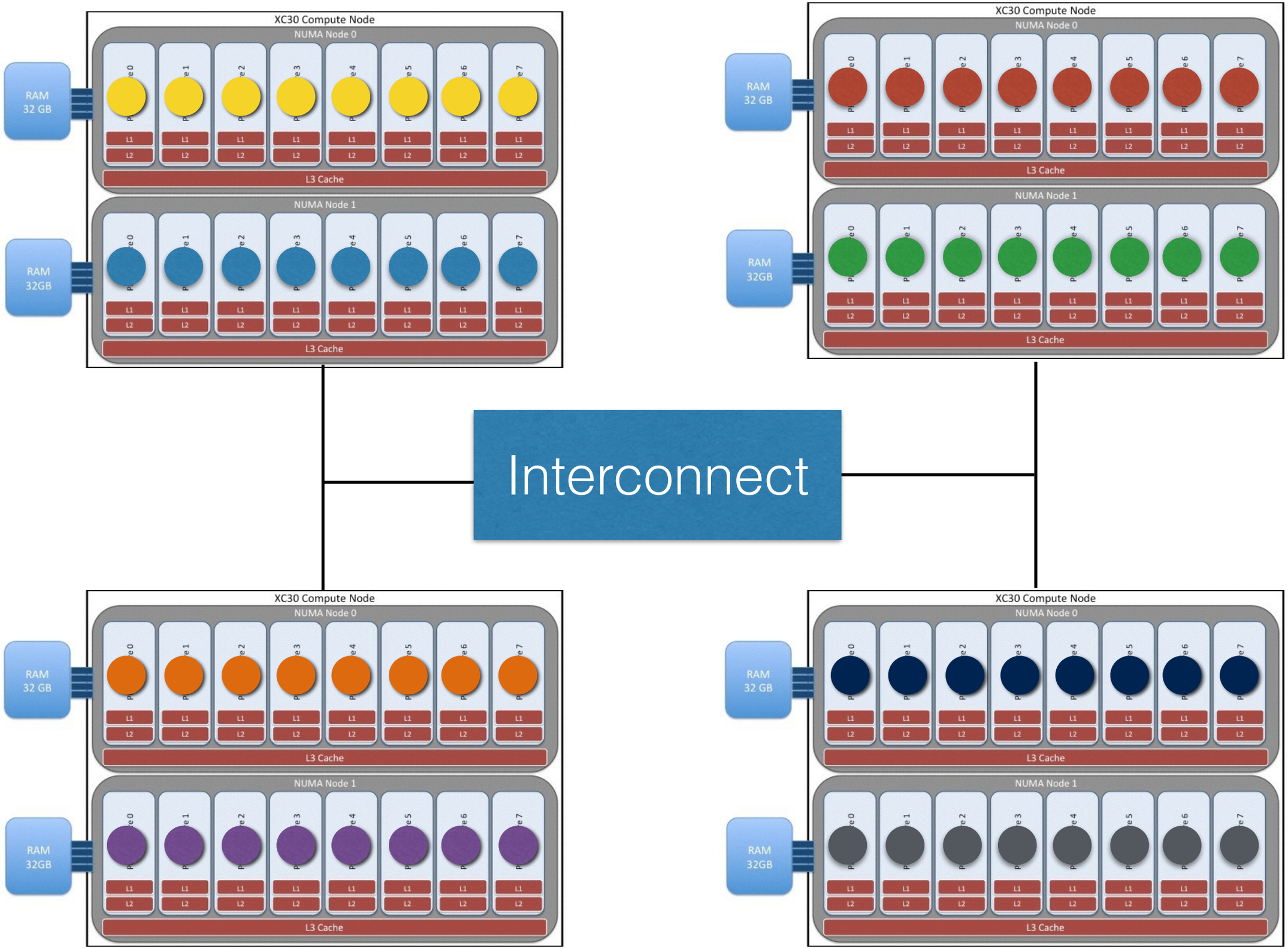
1 MPI task per socket, 8 threads each

```
OMP_NUM_THREADS=4 mpiexec -np 4 ../src/lmp_openmpi-omp -sf omp
```



Core 2 MPI tasks per socket, 4 threads each

OMP_NUM_THREADS=8 mpiexec -npersocket 1 ../src/lmp_openmpi-omp



OpenMP-OpenMPI Hybrid Considerations

- The best parallel efficiency from omp styles is typically achieved when there is at least one MPI task per physical processor, i.e. socket or die.

- Using multi-threading is most effective under the following circumstances:

  - Individual compute nodes have a significant number of CPU cores but the CPU itself has limited memory bandwidth

  - The interconnect used for MPI communication is not able to provide sufficient bandwidth for a large number of MPI tasks per node.

    http://lammps.sandia.gov/doc/Section_accelerate.html#acc_5

OpenMP-OpenMPI Hybrid Considerations

- The input is a system that has an inhomogeneous particle density which cannot be mapped well to the domain decomposition scheme that LAMMPS employs.

- Finally, multi-threaded styles can improve performance when running LAMMPS in "capability mode", i.e. near the point where the MPI parallelism scales out.

http://lammps.sandia.gov/doc/Section_accelerate.html#acc_5