Steps:

I. Load already uploaded modules
   module load apps libs cports

II. Check available modules
   module avail

III. Load modules required
   a. module load default-gcc-openmpi
   b. module load default-intel-openmpi
   c. module load libs mkl/64/11.0.074
   d. module load libs acml/64/gfortran/4.3.0
   e. module load opnempi/1.6.5-gnu4.8.2

IV. List the modules loaded
   module list
      i. cports
      ii. gcc/4.8.2-gnu
      iii. openmpi/1.6.5-gnu4.8.2
      iv. libs
      v. mkl/64/11.0.074
      vi. default-gcc-openmpi
      vii. intel/12.1/composer_xe_2011_sp1.9.293
      viii. default-intel-openmpi
      ix. acml/64/gfortran/4.3.0
      x. apps
      xi. cports6
      xii. intel/12.1/opnempi/64/1.6.5

V. Clean the older data
   a. make arch=lonsdale_gcc493_openmpi186_acml430 clean arch all
   b. make arch=lonsdale_gcc493_openmpi186_mkl11 clean arch all
   c. make arch=lonsdale_intel12_openmpi186_acml430 clean arch all
   d. make arch=lonsdale_intel12_openmpi186_mkl11 clean arch all

VI. Create “Make.arch” files
   a. Make.lonsdale_gcc493_openmpi186_acml430
   b. Make.lonsdale_gcc493_openmpi186_mkl11
   c. Make.lonsdale_intel12_openmpi186_acml430
   d. Make.lonsdale_intel12_openmpi186_mkl11

VII. Make the files
   a. make arch=lonsdale_gcc493_openmpi186_acml430
   b. make arch=lonsdale_gcc493_openmpi186_mkl11
   c. make arch=lonsdale_intel12_openmpi186_acml430
   d. make arch=lonsdale_intel12_openmpi186_mkl11

VIII. Check the .dat and xml files in the bin folder
   a. Four folders created inside bin folder
   b. Two files in each folder
      i. HPL.dat
      ii. Xhpl

IX. Test Run
   a. mpirun -np 8 xhpl
   b. Results:
      T/V : Wall time / encoded variant.
      N : The order of the coefficient matrix A.
      NB : The partitioning blocking factor.
      P : The number of process rows.
      Q : The number of process columns.
      Time : Time in seconds to solve the linear system.
      Gflops : Rate of execution for solving the linear system.

X. Change parameters
   a. More sensitive parameters -> N, NB, P, Q

   b. N: The problem Size
      Use 80% of available RAM
      (8 cores x N x N) = 80% x 16GB = 12.8 x 2^{30}
      ⇨ N = 41448

   c. NB: The problem size
      From a data distribution point of view, the smallest NB, the better the load balance. From a computation point of view, a too small value of NB may limit the computational performance by a large factor because almost no data reuse will occur in the highest level of the memory hierarchy. The number of messages will also increase. Efficient matrix-multiply routines are often internally blocked. The bottom line is that "good" block sizes are almost always in the [32...256] interval. The best values depend on the computation / communication performance ratio of your system

   d. P x Q: The process grid
      Lonsdale has 8 cores
      ⇨ P = 2
      ⇨ Q = 4

XI. Shell scripts for running
   a. bashRunGccMKL.sh
   b. bashRunGccACML.sh
   c. bashRunIccMKL.sh
   d. bashRunIccACML.sh

XII. Run for optimization
   a. Ran for various values of N, NB, P & Q
   b. Best results are shown in the below table

XIII. Store in output files

a. sh bashRunGccMKL.sh >> output.txt
b. sh bashRunGccACML.sh >> output.txt
c. sh bashRunIccMKL.sh >> output.txt
d. sh bashRunIccACML.sh >> output.txt

XIV. Relevant files/folders(created/edited) for the assignment:

a. Makefiles edited for compilation

Make.lonsdale_gcc493_openmpi186_acml430
Make.lonsdale_gcc493_openmpi186_mkl11
Make.lonsdale_intel12_openmpi186_acml430
Make.lonsdale_intel12_openmpi186_mkl11

b. Will have the bash script for getting the results

bashRun.sh

c. Will have compilation results

bin/lonsdale_gcc493_openmpi186_acml430/
bin/lonsdale_gcc493_openmpi186_mkl11/
bin/lonsdale_intel12_openmpi186_acml430/
bin/lonsdale_intel12_openmpi186_mkl11/

d. Slurm files were created for each sbatch run

RESULTS:

ARCH name	lonsdale_gcc493_openmpi186_acml430	lonsdale_gcc493_openmpi186_mkl11	lonsdale_intel12_openmpi186_acml430	lonsdale_intel12_openmpi186_mkl11
Compiler Name	GCC	GCC	ICC	ICC
Compiler Name Version	4.9.3	4.9.3	12.1	12.1
BLAS Library Name	ACML	MKL	ACML	MKL
BLAS Library Name Version	4.3.0	11	4.3.0	11
OpenMPI Version	1.8.6			
T/V	WR00C2R2	WR00L2R2	WR00R2C4	WR00L2L2
N	41000	41000	41472	41000
NB	102	88	88	88
P	2	2	2	2
Q	4	4	4	4
Time	826.44	809.94	796.27	809.67
Gflops	55.6	56.73	59.72	56.75
File	bin/lonsdale_gcc493_openmpi186_acml430/output.txt	bin/lonsdale_gcc493_openmpi186_mkl11/output.txt	slurm-263190.out	slurm-263191.out