MUMPS

workshop 26 Sep 2014

MUMPS

- **MU**ltifrontal **M**assively **P**arallel **S**olver : **MUMPS**
- Package for solving large linear systems:

$$\mathbf{A}\,\mathbf{x} = \mathbf{b}$$

From $\mathbf{Ap} = \mathbf{s}$
Find **LU** that

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{bmatrix}.$$

Then we can obtain **p** from

$$\mathbf{Ly} = \mathbf{s}$$
$$\mathbf{Up} = \mathbf{y}$$

$$(\mathbf{LU})[\mathbf{p}_1, \mathbf{p}_2, \ldots, \mathbf{p}_N] = [\mathbf{s}_1, \mathbf{s}_2, \ldots, \mathbf{s}_N]$$

Required Package

- BLAS
- BLACS
- LAPACK
- SCALARPACK
- MPI

- ip : 10.9.76.123

- > sftp 10.9.76.123
- > cd /home/physics/
- > get mumps_tutorial.tgz
- > tar xzvf mumps*
- > cd mump…
- >

BLAS

- cd BLAS
- vi make.inc

- make all

```
####################################################################
#  BLAS make include file.                                         #
#  March 2007                                                      #
####################################################################
#
SHELL = /bin/sh
#
#  The machine (platform) identifier to append to the library names
#
PLAT = _LINUX
#
#  Modify the FORTRAN and OPTS definitions to refer to the
#  compiler and desired compiler options for your machine.  NOOPT
#  refers to the compiler options desired when NO OPTIMIZATION is
#  selected.  Define LOADER and LOADOPTS to refer to the loader and
#  desired load options for your machine.
#
FORTRAN  = gfortran
OPTS     = -O3
DRVOPTS  = $(OPTS)
NOOPT    =
LOADER   = gfortran
LOADOPTS =
#
#  The archiver and the flag(s) to use when building archive (library)
#  If you system has no ranlib, set RANLIB = echo.
#
ARCH     = ar
ARCHFLAGS= cr
RANLIB   = ranlib
#
#  The location and name of the Reference BLAS library.
#
BLASLIB      = libblas.a
~
```

BLACS

```
>  gunzip -c mpiblacs.tgz | tar xf -
>  gunzip -c blacstester.tgz | tar xf -
>  gunzip -c mpiblacs-patch03.tgz | tar xf -
>  cd BLACS
>  cp BMAKES/Bmake.MPI-LINUX Bmake.inc
>  vi Bmake.inc

        SHELL = /bin/bash
        BTOPdir = /home/physics/Desktop/Mworkshop/BLACS
        BLACSFINIT  = $(BLACSdir)/libblacsF77init.a
        BLACSCINIT  = $(BLACSdir)/libblacsCinit.a
        BLACSLIB    = $(BLACSdir)/libblacs.a
        MPIdir = /opt/mpich3
        TRANSCOMM = -DCSameF77
        F77             = mpif77
        CC              = mpicc

> esc + :wq
> make all
```

LAPACK

```
>  tar -xf lapack-3.4.2.tar
>  cp make.inc.example make.inc
>  vi make.inc
        SHELL = /bin/bash
        FORTRAN  = mpif90
        LOADER   = mpif90
        CC = mpicc
        BLASLIB      = /home/physics/Desktop/Mworkshop/BLAS/libblas.a

> esc + :wq
> make all
```

SCALARPACK

```
 >  tar -xf scalapack-2.0.2.tar
 >  cp SLmake.inc.example SLmake.inc
 >  vi SLmake.inc

           BLASLIB       = /home/physics/Desktop/Mworkshop/BLAS/libblas.a
           LAPACKLIB     = /home/physics/Desktop/Mworkshop/lapack-3.4.2/
liblapack.a

 > esc + :wq
 > make all
```

SCALARPACK

```
 >  tar -xf scalapack-2.0.2.tar
 >  cp SLmake.inc.example SLmake.inc
 >  vi SLmake.inc

          BLASLIB       = /home/physics/Desktop/Mworkshop/BLAS/libblas.a
          LAPACKLIB     = /home/physics/Desktop/Mworkshop/lapack-3.4.2/
liblapack.a

 > esc + :wq
 > make all
```

MUMPS

```
>  tar -xf MUMPS_4-1.10.0.tar
>  cd MUMPS_4.10.0
>  cp Make.inc/Makefile.inc.generic ./Makefile.inc
>  vi Makefile.inc

     topdir    = /home/physics/Desktop/Mworkshop/MUMPS_4.10.0
     CC      = mpicc
     FC      = mpif90
     FL      = mpif90
     SCALAP  = /home/physics/Desktop/Mworkshop/scalapack-2.0.2/
   libscalapack.a /home/physics/Desktop/Mworkshop/BLACS/LIB/libblacs.a /home/
   physics/Desktop/Mworkshop/BLACS/LIB/libblacsCinit.a /home/physics/Desktop/
   Mworkshop/BLACS/LIB/libblacsF77init.a /home/physics/Desktop/Mworkshop/
   lapack-3.4.2/liblapack.a
      INCPAR  = -I/opt/mpich3/include
      LIBBLAS = /home/physics/Desktop/Mworkshop/BLAS/libblas.a

>  esc + :wq
>  make all
```

Main Steps

1. Analysis / Preprocessing : $\mathbf{A_{pre}}$
2. Factorization : $\mathbf{A_{pre} = LU}$ or $\mathbf{LDL^T}$
3. Solution

MUMPS versions

- **S : Real**
- **D : Double precision**
- **C : Complex**
- **Z : Complex double**

Test script