

Parallel processing and matrix solver interface: mt xp

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Notice

- Version number of the software in the following will change owing to updates of the software.

1 Parallel processing library: MPICH

1.1 Download

1. Download a source file from MPICH web:

[https://www.mpich.org/downloads/
mpich-3.3.1.tar.gz](https://www.mpich.org/downloads/mpich-3.3.1.tar.gz) (26MB)

2. Make a directory and expand the source file

```

cd
mkdir soft
cd soft
mkdir mpich
cd mpich
mv ~/Download/mpich-3.3.1.tar.gz .
tar xzf mpich-3.3.1.tar.gz
cd mpich-3.3.1

```

1.2 Configure

1. Create a configure script “run” by your favorite editor

run:

```

CC=gcc CFLAGS="-m64" CXX=c++ CXXFLAGS="-m64" FC=gfortran
FFLAGS="-m64" ./configure --prefix=/usr/local/mpich331-gfortran-gcc
--enable-cxx --enable-fast --enable-romio --disable-shared

```

- One line text (no new line in the file)
- Install directory is defined as /usr/local/mpich331-gfortran-gcc

2. Make “run” executable

```

chmod 755 run

```

3. Configure

```

./run

```

1.3 Compile and install

1. Compile

```

make

```

2. Install

```

sudo make install

```

2 Parallel matrix solver library: PETSc

2.1 Download

1. Download a source file from PETSc web site

```

https://www.mcs.anl.gov/petsc/download/
petsc-3.11.3.tar.gz (33.2MB)

```

2. Make a directory and expand the source file

```

sudo mkdir /opt
cd /opt
sudo mkdir petsc
sudo chown admin:admin petsc \quad ("admin" should be replaced by you

```

```

user name)
cd petsc
mv ~/Download/petsc-3.11.3.tar.gz .
tar xzf petsc-3.11.3.tar.gz

```

2.2 Configure

1. Create a configure script “gfortran.py” by your favorite editor

```

gfortran.py

#!/usr/bin/env python

# Build PETSc, with gfortran

configure_options = [
    '--with-mpi=1',
    '--with-mpi-dir=/usr/local/mpich331-gfortran-gcc',
    '--with-shared-libraries=0',
    '--with-cxx-dialect=C++11',
    '--download-mpich=0',
    '--download-hypre=0',
    '--download-fblaslapack=1',
    '--download-spooles=1',
    '--download-superlu=1',
    '--download-metis=1',
    '--download-parmetis=1',
    '--download-superlu_dist=1',
    '--download-blacs=1',
    '--download-scalapack=1',
    '--download-mumps=1'
]

if __name__ == '__main__':
    import sys,os
    sys.path.insert(0,os.path.abspath('config'))
    import configure
    configure.petsc_configure(configure_options)

```

2. Make “gfortran.py” executable

```

chmod 755 gfortran.py

```

3. Setup environment variables for PETSc

```

export PETSC_DIR=/opt/petsc/petsc-3.11.3
export PETSC_ARCH=gfortran

```

4. Configure

```

./gfortran.py

```

5. Make a soft link to prepare for library updates

```

sudo ln -s petsc-3.11.3 petsc

```

2.3 Compile

1. Compile

```
make all
```

3 Compile of task/mtxp module

3.1 Setup make.mtxp file

1. Goto mtxp directory

```
cd task/mtxp
```

2. Create a setup file

```
cp make.mtxp.org make.mtxp
```

3. Edit the setup file “make.mtxp”

- If MPI is not available, remove comment mark “#” on lines 4–9
- If MPI is available but PETs not, remove comment mark “#” on lines 12–17
- If MPI and PETSc are available, remove comment mark “#” on lines 21, 38,39, 41–45

3.2 Modify make.header file

1. Go to task directory

```
cd ..
```

2. Edit make.header to use lapack and blas libraries for fortran

- Near the beginning of the file, remove comment and adjust the path

```
LAPACK = lapack.f
LIBLA=-L /opt/PETSc/petsc/gfortran/lib -llapack -lblas
```
- In the following, add comment marks

```
#LAPACK = nolapack.f
#LIBLA =
MODLA95 =
Keep MODLA95 as it is, since lapack95 is not used.
```
- Go back to mtxp directory

```
cd mtxp
```

3.3 Compile

1. Compile

```
make clean
make
```

3.4 Test mt xp

1. Test programs solving 1d, 2D and 3D diffusion equation are generated

- `testbnd`: Direct band matrix solver (non-parallel)
- `testpcg`: Iterative band matrix solver (non-parallel)
- `testdmumps`: Direct band matrix solver (parallel using MUMPS)
- `testkdsp`: Iterative band matrix solver (parallel using PETSc)

2. Input parameters

- `idimen` : number of dimension (1 or 2 or 3), 0 for quit
- `isiz` : number of mesh point in one dimension
- `isource` : source position in all dimensions
- `itype` : type of initial guess for PETSc 0..5 (default=0)
- `m1` : type of solver (methodKSP) of PETSc 0..13 (default=4)
- `m2` : type of preconditioner (methodPC) 0..12 (default=5)
- `tolerance` : tolerance in iterative method

3. Example input For parallel processing

```
mpirun -np 4 ./testdmumps
# INPUT: idimen,isiz,isource,itype,m1,m2,tolerance,idebug=
1,11,6,0,4,5,1.D-7
3/
0/
```

4 Compile of task/fp and related modules

4.1 Update Makefile

1. Change directory

```
cd ../fp
```

2. Edit Makefile

- To use serial band matrix solver, remove comment mark “#” on lines 4-5.
- To use serial iterative solver, remove comment mark “#” on lines 6-7.
- To use parallel direct solver MUMPS, remove comment mark “#” on lines 8-9.
- To use parallel direct solver library PETSc, remove comment mark “#” on lines 10-11. .

4.2 Compile

1. Compile related modules and task/fp files

```
make
```

5 Install on Ubuntu

5.1 Install of required modules

```
sudo apt-get install gfortran-8
sudo apt-get install gcc-8
sudo apt-get install g++-8
```

```
sudo apt-get install emacs
sudo apt-get install git
sudo apt-get install xorg-dev
sudo apt-get install valgrind
sudo apt-get install cmake
sudo apt-get install python
```

5.2 Install of MPICH

1. Download of mpich-3.3.1.tar.gz (See 1.1)
2. Expand at /soft/mpich (See 1.1)
3. Configure by executing “./run” (See 1.2)

run:

```
CC=gcc-8 CFLAGS='-m64' CXX=g++-8 CXXFLAGS='-m64' FC=gfortran-8
FFLAGS='-m64' ./configure --prefix=/usr/local/mpich331-gfortran-gcc8
--enable-cxx --enable-fast --enable-romio --disable-shared
```

4. Compile and install (See 1.3)

5.3 Install of PETSc

1. Download of petsc-3.11.3.tar.gz (See 2.1)
2. Expand at /opt/PETSc/ (See 2.1)
3. Setup environment variables (See 2.2)

```
export PETSC_DIR=/opt/PETSc/petsc-3.11.3
export PETSC_ARCH=gfortran
```

4. Configure by gfortran.py (See 2.2)
5. Execute fortran.py

gfortran.py:

```
#!/usr/bin/env python

# Build PETSc, with gfortran

configure_options = [
    '--with-mpi=1',
    '--with-mpi-dir=/usr/local/mpich331-gfortran-gcc8',
    '--with-shared-libraries=0',
```

```

'--with-cxx-dialect=C++11',
'--download-mpich=0',
'--download-hypre=0',
'--download-fblaslapack=1',
'--download-spooles=1',
'--download-superlu=1',
'--download-metis=1',
'--download-parmetis=1',
'--download-superlu_dist=1',
'--download-blacs=1',
'--download-scalapack=1',
'--download-mumps=1'
]

if __name__ == '__main__':
    import sys,os
    sys.path.insert(0,os.path.abspath('config'))
    import configure
    configure.petsc_configure(configure_options)

```
