2019-09-28

Parallel processing and matrix solver interface: mtxp

Contents

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 (26MB)
   ```

2. Make a directory and expand the source file

   ```
   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 favarite editor

   ```
   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
   ```

   Install directory: `/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 \qquad ("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 favarite editor

```
#!/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
```

2.3 Compile

1. Compile

```
make all
```

3 Compile of task/mtxp module

3.1 Update setup 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 Compile

1. Compile

```
make
```

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
   ```