How to install the integrated code: TASK

A. Fukuyama
Professor Emeritus, Kyoto University

1. Preparation for macOS

2. In case of macOS major version up

3. Preparation for Ubuntu

4. Introduction to git

5. Install task and related libraries

6. Introduction to the task code

7. Install PETSc

Preparation for macOS (1)

- **Install Xcode**

    – Xcode: development environment on macOS

    – Use App Store

    – Category: Development

    – Choose and install Xcode

- **Install Command_Line_Tools**

    – Command_Line_Tools: various Unix commands for development

    – Input command on terminal

    – `xcode-select --install`

- **Install XQartz**

    – Download and install XQartz from https://www.xquartz.org

- **Install java**

    – Download and install java from
    https://www.java.com/en/download/mac_download.jsp

Preparation for macOS (2)

- **Install Macports**

  - Download the latest macports binary from https://www.macports.org
  - Select tab: Installing MacPorts
  - Quickstart: download and install MacPorts installer for appropriate macOS version
  - MacPorts is mostly installed at /opt/local
  - Update to the latest Macports

    - `sudo port selfupdate`
    - `sudo port upgrade outdated`

- **Install compiler and related modules**

  - gfortran: `sudo port install gcc12`
  - mpich: `sudo port install mpich`
  - others: `sudo port install gmake cmake imake`

In case of macOS major version-up

- **macOS major version-up**: e.g. 13.3 $\implies$ 14.0

- **Update Xcode**

  – Use App Store to update Xcode

- **Update Command_Line_Tools**

  – `xcode-select --install`

- **Update Macports**

  – Download and install the Macports binary for the new version of macOS from https://www.macports.org

  – It may take a few days before the binary for the new version of macOS becomes available.

  – Update the installed ports to the new Macports binary

    ◦ `sudo port selfupdate`

    ◦ `sudo port upgrade outdated`

Preparation for Ubuntu

1. **Install required modules**

   ```
   sudo apt-get install gfortran-12
   sudo apt-get install gcc-12
   sudo apt-get install g++-12

   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

   sudo apt-get install mpich
   ```

How to use git (1)

- **git**: version and remote repository control facility
- **Repositories**
  - **local**: in your machine
  - **remotes**: in remote servers
  - **remotes**/**origin**: in default server: bpsi.nucleng.kyoto-u.ac.jp
- **Branches**
  - **There are several branches for code development**
    - ○ **master**: default, stable version, often rather old
    - ○ **develop**: latest version, where I am working
    - ○ **others**: branches for working specific modules
  - cd task
  - git branch   : list branch names, local only
  - git branch -a   : list branch names, local and remote

How to use git (2)

- **To use develop branch**

  – **Create local branch develop and associate it with remote develop**

  – git checkout -t -b develop origin/develop

  – git branch

- **Change working branch**

  – git checkout master

  – git checkout develop

- **Update working branch**: download from remote repository

  – git pull

    ◦ Your modification is kept, if committed.

    ◦ If uncommitted modification remains, no overwrite.

    ◦ use git stash to keep away your modification.

    ◦ If there are conflicts with your committed modification, the conflicts are indicated in the file. Correct them and git pull again.

How to use git (3)

- **To check your modification**

  – git status

- **To commit your modification with message**: only local depository is updated. message is required.

  – git commit -a -m'*message*'

- **To list all modification**

  – git log

- **To show difference from committed repository**

  – git diff [*filename*]

- **For more detail, visit**

  – https://git-scm.com/documentation

Install TASK (1)

- **Check availability of git**: just command input "git"

- **Set your identity**: To record who changed the code?

  – git config - -global user.name "[your-full-name]"

  – git config - -global user.email [your-mail-address]

  – For example,

    ◦ git config - -global user.name "Atsushi Fukuyama"

    ◦ git config - -global user.email fukuyama@nucleng.kyoto-u.ac.jp

  – Data is saved in $HOME/.gitconfig

- **Create a working directory**: any directory name is OK

  – mkdir git

  – cd git

Install TASK (2)

- **Download TASK and necessary libraries** for download only
  - git clone https://bpsi.nucleng.kyoto-u.ac.jp/pub/git/gsaf.git
  - git clone https://bpsi.nucleng.kyoto-u.ac.jp/pub/git/bpsd.git
  - git clone https://bpsi.nucleng.kyoto-u.ac.jp/pub/git/task.git
- **Download TASK and necessary libraries** for download and upload
  - git clone ssh://username@bpsi.nucleng.kyoto-u.ac.jp/pub/git/gsaf.git
  - git clone ssh://username@bpsi.nucleng.kyoto-u.ac.jp/pub/git/bpsd.git
  - git clone ssh://username@bpsi.nucleng.kyoto-u.ac.jp/pub/git/task.git
  - username@ can be omitted if the usernames at remote and local are same.
- **Three directories are created**
  - **gsaf**: graphic library
  - **bpsd**: data interface library
  - **task**: main TASK directory

Install TASK (3)

- **Install graphic library GSAF**

  – cd git/gsaf/src

  – Copy Makefile.arch appropriate for your environment

    ◦ for macOS: cp ../arch/macos-gfortran/Makefile.arch .

    ◦ for Ubuntu: cp ../arch/ubuntu-gfortran64-static/Makefile.arch .

  – **Edit Makefile.arch**: adjust BINPATH and LIBPATH to available ones

    ◦ BINPATH: graphic commands are located, should be included in $PATH in ~/.profile or ./zprofile

    ◦ LIBPATH: graphic libraries are located, should be included in library path for compiling applications using the graphic libs.

  – make

  – make install

    ◦ if BINPATH is protected, use "sudo make install"

Install TASK (4)

- **Check the availability of GSAF library**

  - cd test

  - make

  - Applications using GSAF library must be started from X11 window such as xterm, not from Terminal on macOS.

  - ./bsctest

  - 5   : Choose the size of window

  - c   : Continue the run

  - m

  - New graphic window opens and marks and lines are drawn.

  - To go back to the original window, enter CR.

  - If focus does not change, click the original window and check XQartz preferences.

  - e   : Close the graphic window

  - cd ../../..

Install TASK (5)

- **Use the latest develop branch and setup files, make.header and make.mtxp**

  - cd task

  - git checkout -t -b develop origin/develop

  - cp make.header.org make.header

  - **Edit make.header** to remove comments for target OS and compiler

- **Compile data exchange library BPSD**

  - cd ../bpsd

  - make

  - cd ../task

Install TASK (6)

- **Choice of matrix solver configuration**

  – Single processing without MPI: make.mtxp.nompi

  – Single processing with MPI: make.mtxp.mpi

  – Multi processing with parallel real matrix solver: make.mtxp.petsc

  – Multi processing with parallel real and complex solver: make.mtxp.petsc+mumps

- **Module using parallel matrix solver**

  – **Real**: fp, ti, pic, t2

  – **Complex**: wmx, wf2d, wf2dt, wf2dx, wq

- **Setup matrix solver library**

  – cd mtxp

  – cp make.mtxp.XXX make.mtxp

  – make

  – cd ..

- **Compile modules**:
  - cd lib
  - make
  - cd ..
- **Compile and run TASK module**: eq for example
  - cd eq
  - make
  - ./eq
  - 5
  - c
  - r
  - g
  - s, CR, CR, $\cdots$
  - x
  - q

How to use GSAF

- **At the beginning of the program**

  - **Set graphic resolution** (0: metafile output only, no graphics)
  - **commands**
    - **c**: continue
    - **f**: set metafile name and start saving

- **At the end of one page drawing**

  - **commands**
    - **c** or **CR**: change focus to original window and continue
    - **f**: set metafile name and start saving
    - **s**: start saving and save this page
    - **y**: save this page and continue
    - **n**: continue without saving
    - **d**: dump this page as a bitmap file "gsdump*n*"
    - **b**: switch on/off bell sound
    - **q**: quit program after confirmation

Graphic Utilities

- **Utility program**

  - **gsview**: View metafile
  - **gsprint**: Print metafile on a postscript printer
  - **gstoeps**: Convert metafile to eps files of each page
  - **gstops**: Convert metafile to a postscript file of all pages
  - **gstotgif**: Convert metafile to a tgif file for graphic editor tgif
  - **gstotsvg**: Convert metafile to a svg file for web browser

- **Options**

  - **-a**: output all pages, otherwise interactive mode
  - **-s ps**: output from page ps
  - **-e pe**: output until page pe
  - **-p *np***: output contiguous *np* pages on a sheet
  - **-b**: output without title
  - **-r**: rotate page
  - **-z**: gray output

Typical File Name of TASK

- `XXcomm.f90`: Definition of global variables, allocation of arrays

- `XXmain.f90`: Main program for standalone use, read XXparm file

- `XXmenu.f90`: Command input

- `XXinit.f90`: Default values

- `XXparm.f90`: Read input parameters

- `XXview.f90`: Show input parameters

- `XXprep.f90`: Initialization of run, initial profile

- `XXexec.f90`: Execution of run

- `XXgout.f90`: Graphic output

- `XXfout.f90`: Text file output

- `XXsave.f90`: Binary file output

- `XXload.f90`: Binary file input

Typical input command

- When input line includes `=`, interpreted as a namelist input (e.g., `rr=6.5`)
- When the first character is not an alphabet, interpreted as line input
- `r`: Initialize profiles and execute
- `c`: Continue run
- `p`: Namelist input of input parameters
- `v`: Display of input parameters
- `s`: Save results into a file
- `l`: Load results from a file
- `q`: End of the program
- **Order of input parameter setting**
  - Setting at the subroutine `XX_init` in `XXinit.f90`
  - Read a namelist file `XXparm` at the beginning of the program
  - Setting by the input line

Install PETSc (1)

- **PETSc**: Parallel matrix solver library

  - blas,lapack: matrix solver tolls
  - scalapack, metis, parmetis, blacs, superlu: parallel solver tools
  - MUMPS: Direct matrix solver for real and complex
  - PETSc: Iterative matrix solver for real or complex

- **Make PETSc directory and change its owner**

  - `sudo mkdir /opt/PETSc`

  - `sudo chown /opt/PETSc $USERNAME`

  - `cd /opt/PETSc`

- **Download latest PETSc library package by git**

  - **First download of PETSc source**

    ○ `git clone -b release https://gitlab.com/petsc/petsc.git petsc`

  - **In order to update PETSc source**

    ○ `git pull`

Install PETSc (2)

- **Provide environment variables for PETSC in ~/.profile or .zprofile**
  - `export PETSC_DIR=/opt/PETSc/petsc`
  - `export PETSC_ARCH=default`
- **Configure script in python**
  - **Copy `default.py` to `/opt/PETSc/petsc`**
  - **Provide exec attribute to `default.py`**
    - `chmod 755 default.py`
  - **Execute configuration script**   (It may take half an hour.)
    - `./default.py`
  - **Additional libraries are created in default/externalpackages**
- **Make and check PETSc library**
  - `make`   (It may take half an hour.)
  - `make check`