FrontISTR Installation Manual

FrontISTR Commons

$July\ 29,\ 2019$

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1 FrontISTR Installation Manual

This software is the outcome of "Research and Development of Innovative Simulation Software" project supported by Research and Development for Next-generation Information Technology of Ministry of Education, Culture, Sports, Science and Technology. We assume that you agree with our license agreement of "MIT License" by using this software either for the purpose of profit-making business or for free of charge. This software is protected by the copyright law and the other related laws, regarding unspecified issues in our license agreement and contact, or condition without either license agreement or contact.



| Item | Content |
|----------------------|---------------------------|
| Name of Software | FrontISTR |
| Version | 5.0 |
| License | MIT License |
| Correnponding Clerks | FrontISTR |
| | Commons2-11-16 |
| | Yayoi, Bunkyo-ku, |
| | Tokyoc/o Institute |
| | of Engineering |
| | Innovation, School |
| | of EngineeringE- |
| | mail support@frontistr.co |

1.1 Manuals

- Introduction
- How to install
- Theory
- User's manual
- Tutorial

This manual explains the installation procedure for a large-scale structural analysis program using the finite element method (FEM), FrontISTR.

1.2 List of description on this manual

- Installation
- Required software
- Extracting the Archive File
- Installation
- Compile with cmake
 - Example of installation procedure to CentOS7.6 (cmake)

- Example of installation procedure to Ubuntu18.04 (cmake)
- Compile with editing Makefile.conf manually
 - List of Makefile.conf Variables
 - Example of installation procedure to CentOS7.6 (Makefile.conf)
 - Example of installation procedure to Ubuntu18.04 (Makefile.conf)
 - Example of installation procedure to Windows10 (Makefile.conf)

1.3 Operating Environment

1.3.1 Required software

To install this software, the following software programs must have been installed in the environment where this software is to be installed. For information on how to install these software programs, refer to their installation manuals.

1.3.1.1 C, C++ and Fortran90 compilers

C, C++, and Fortran90 compilers are required to install this software.

1.3.1.2 MPI

This software executes parallel processing via MPI and requires an MPI library that compiles with the MPI-1 standards. Representative free-of-charge libraries that implement MPI include MPICH and OpenMPI. OpenMPI and MPICH can be downloaded from the following website:

Open MPI: Open Source High Performance Computing

• https://www.open-mpi.org/

High-Performance Portable MPI

• http://www.mpich.org/

1.3.1.3 METIS

The domain decomposition utilities of this software use the METIS libraries to enable domain decomposition using pMETIS and kMETIS. METIS is required to use these domain decomposition functions. Supported versions of METIS are the newest version Ver.5 series and previous version Ver.4 series.

For environments where METIS is not installed, domain decomposition is still possible using the RCB algorithm.

METIS - Serial Graph Partitioning and Fill-reducing Matrix Ordering

• http://glaros.dtc.umn.edu/gkhome/metis/metis/overview

1.3.1.4 ParMETIS

We plan to use the ParMETIS library as the parallel domain decomposition utilities for this software.

ParMETIS is not required at present.

ParMETIS - Parallel Graph Partitioning and Fill-reducing Matrix Ordering

• http://glaros.dtc.umn.edu/gkhome/metis/parmetis/overview

1.3.1.5 HEC-MW

This software uses the HEC-MW library developed by the "Revolutionary Simulation Software" and "Research and Development of Innovative Simulation Software" projects.

HEC-MW comes bundled with the FrontISTR archive file, and is automatically compiled when this software is installed, so there is no need to install HEC-MW separately.

1.3.1.6 REVOCAP_Refiner

This software is compatible with the REVOCAP_Coupler coupled analysis tool developed by the "Research and Development of Innovative Simulation Software" project. REVOCAP_Coupler is required to use the coupled analysis function. REVOCAP_Coupler can be downloaded from the following website:

• http://www.multi.k.u-tokyo.ac.jp/FrontISTR/

1.3.1.7 REVOCAP Coupler

This software is compatible with the REVOCAP_Coupler coupled analysis tool developed by the "Research and Development of Innovative Simulation Software" project.REVOCAP_Coupler is required to use the coupled analysis function. REVOCAP Coupler can be downloaded from the following website:

• http://www.ciss.iis.u-tokyo.ac.jp/dl/index.php

1.3.1.8 LAPACK/BLAS

This software is implemented a function of estimating condition number of preconditioned matrix.

When you use this function, LAPACK and BLAS libraries are required.

Reference implements of LAPACK can be downloaded from the following website:

• http://www.netlib.org/lapack/

Reference implements of BLAS can be downloaded from the following website:

• http://www.netlib.org/blas/

OpenBLAS is compatible, fast and Open-Sourced implements of LAPACK/BLAS. OpenBLAS can be downloaded from the following website:

• http://www.openblas.net/

If Intel MKL is installed, it is not necessary to install above software.

1.3.1.9 MUMPS

This software is compatible with a public domain parallel direct solver MUMPS (a MUltifrontal Massively Parallel sparse direct Solver). MUMPS is based on public domain software developed during the Esprit IV European project PARASOL (1996-1999). Since this first public domain version in 1999, research and developments have been supported by the following institutions: CERFACS, CNRS, ENS Lyon, INPT(ENSEEIHT)-IRIT, INRIA, and University of Bordeaux. MUMPS can be downloaded from the following website:

• http://mumps.enseeiht.fr/

1.3.1.10 ScaLAPACK

Therefore this software doesn't use this directly, MUMPS needs ScaLAPACK for compiling. ScaLAPACK can be downloaded from the following website:

• http://www.netlib.org/scalapack/

If Intel MKL is installed, it is not necessary to install above software.

1.3.1.11 ML

This software is compatible with multigrid preconditioner package ML (Multi-Level Preconditioner). ML is one of the packages developed under Trilinos project at Sandia National Laboratories. ML can be downloaded from the following website:

• https://trilinos.org/

1.3.1.12 Intel MKL Math Kernel Library

The contact analysis module of this software uses Intel MKL. If Intel MKL has not been installed in the environment where this software is to be installed, some of the contact analysis functions cannot be used.

1.3.2 Operation verification environment

Operations of this software have been verified in the following environment. However, if the software programs (described above) required for installing this software have been installed, this software should operate normally even in environments other than the environment shown below.

1.3.2.1 Operation verification environment

| System | Operatingsystem | CPU | Compiler | Parallel processingenvironment |
|-----------------------|--------------------------------------|------------------------|----------------------|--------------------------------|
| K computer | Linux | SPARC64 VIIIfx | Fujitsu compiler | Fujitsu MPI |
| PRIMEHPC FX100 | Linux | SPARC V9 + HPC-ACE2 | Fujitsu compiler | Fujitsu MPI |
| EARTH SIMULATOR(ES | SUPER UX 53) | SX-ACE | NEC compiler | NEC MPI |
| UV2000 | Linux (SUSE Linux Enterprise 10) | Intel Xeon | Intel compiler | SGI MPT |
| PC cluster | Linux (CentOS-7) | Intel Xeon | Intel compiler | Intel MPI |
| PC cluster | Linux (RedHat Enterprise Linux 7) | Intel Xeon | Intel compiler | OpenMPI |
| Desktop PC | Linux (ubuntu 16.04, 18.04) | AMD Ryzen | GNU compiler | OpenMPI |
| Desktop PC | Linux (ubuntu 16.04, 18.04) | AMD Ryzen | PGI compiler | OpenMPI |
| Desktop PC | Linux (ubuntu 16.04, 18.04) | Intel Core-i7 | GNU compiler | OpenMPI |
| Desktop PC | Windows (7, 10) | Intel Core-i7 | GNU compiler (mingw) | Microsoft MPI |
| Raspberry PI 3 B+ | Linux (raspbian 32bit) | ARM Cortex-A53 | GNU compiler | OpenMPI |
| Notebook PC | macOS Mojave | Intel Core i7 | GNU Compiler | OpenMPI |

1.4 Extracting the Archive File

The archive file has been archiving with the tar command and compressing with gzip. It can be extracted using the following command. ("\$" at the beginning of the command string represents a prompt.)

```
$ tar xzf FrontISTR_V50.tar.gz
```

If the tar command in the environment where this software is to be installed does not support the z option, the archive file can be extracted using the following command:

```
$ gzip -dc FrontISTR_V50.tar.gz | tar xf -
```

If the archive file is extracted, a directory named "FrontISTR" will be created in the directory where the archive file has been extracted. (This directory is hereafter referred to a "\${FSTRBUILDDIR}".)

1.5 Installation

1.5.1 Supported installation procedure

This software supports two procedure for compiling.

1.5.1.1 Compile with cmake

This software supports compiling the software using cmake.

cmake need to be installed in advance. cmake can be downloaded from the following website:

https://cmake.org/

```
$ cd `${FSTRBUILDDIR}`
$ mkdir build
$ cd build
$ cmake ...
$ make -j2
$ make install
```

cmake will search libraries and headers and gererate proper Makefiles for compiling. If you have multi-cored CPU, you will run parallel make for saving compile time.

continue... (Compile with cmake)

1.5.1.1.1 Appendix

- Appendix: Example of installation procedure to CentOS7.6(cmake)
- Appendix: Example of installation procedure to Ubuntu18.04(cmake)

1.5.1.2 Compile with editing Makefile.conf manually

This software supports compiling the software manually edited Makfile.conf.

```
$ cd `${FSTRBUILDDIR}`
$ cp Makefile.conf.org Makefile.conf
$ vi Makefile.conf
    Edit Makefile.conf manually, indicate the location of libraries and headers.
$ ./setup.sh [Options]
$ make
$ make install
```

When difficult to set automatic configuration with cmake, recommend manually editing Makefile.conf.

continue... (Compile with editing Makefile.conf)

1.5.1.2.1 Appendix

- Appendix: Example of installation procedure to CentOS7.6(Makefile.conf)
- Appendix: Example of installation procedure to Ubuntu18.04(Makefile.conf)
- Appendix: Example of installation procedure to Windows10(Makefile.conf)

1.6 Compile with cmake

cmake will find libraries and headers automatically. You can also specify libraries and headers manually.

Detiled usage of cmake command, see https://cmake.org/.

1.6.1 Preparation

In advance, required software install as following directory structure.

```
$HOME
|-- local
|-- bin
|-- include
```

Add \$HOME/local/bin in \$PATH environment variable.

Next, check whether already installed cmake. You may need to install version 2.8.11 or later.

```
$ cmake --version cmake version 2.8.12.2
```

1.6.2 Compiling

Compile FrontISTR.

```
$ cd `${FSTRBUILDDIR}`
$ mkdir build
$ cd build
$ cmake ..
$ make -j2
```

-j2 option follows make command tells make to execute simultaneously. Reduce compile time when increasing the number of simultaneous.

1.6.3 Executing make install

When finished to compile, execute following command.

```
$ make install
```

This software will be installed in the /usr/local/bin directory or in the directory specified by -DCMAKE_INSTALL_PREFIX.

```
$ cmake -DCMAKE INSTALL PREFIX=$HOME/local ...
```

Which options enabled in compiled FrontISTR(fistr1) can confirm as following command.

```
$ ./fistr1 -v
FrontISTR version 5.0.0 (2d3fdb51979459c7ea9357a7c9b790fa69dfd4e2)
MPI: Enabled
OpenMP: Enabled
HECMW_METIS_VER: 5
Compile Option: -p --with-tools --with-metis --with-mumps --with-lapack --with-ml
```

1.6.4 cmake options

You can explicitly various options at configuration time.

| Options | | | | | |
|----------------|--------------------------------------|-------------------|--|--|--|
| (Default) | Contents | Remarks | | | |
| - | Compiling tools such as partitioners | hecmw_part1 etc. | | | |
| DWITH TOOLS=ON | | | | | |
| - | Enable MPI | require libraries | | | |
| DWITH_MPI=ON | | | | | |

| Options (Default) | Contents | |
|-------------------|---------------------------------------|--|
| | Contourns | Remarks |
| - | Enable OpenMP | require supported compiler |
| DWITH_OPENMP | =ON | |
| - | Enable REVOCAP_Refiner | require libraries |
| DWITH_REFINER | fu O :Nonality | |
| - | Enable REVOCAP_Coupler | require libraries |
| DWITH_REVOCAL | Rm@Nonality | |
| - | Enable METIS functionality | 4.0.3 and 5.1.0 supported |
| DWITH_METIS=C | ON | |
| | In case of using metis-4.0.3, specify | In case of using metis-5.1.0, it isn't necessary to |
| DMETIS_VER_4= | O FF | specify it. |
| | Enable ParMETIS functionality | 3.2.0 and 4.0.3 supported |
| DWITH_PARMET | IS=ON | |
| - | In case of using ParMetis-3.2.0, | In case of using parmetis-4.0.3, it isn't necessary to |
| DMETIS_VER_3= | - * | specify it. |
| | Enable MKL PARDISO | require libraries |
| DWITH_MKL=ON | | |
| - | Enable MUMPS functionality | require libraries |
| DWITH_MUMPS= | ON | |
| - | Enable LAPACK functionality | require libraries |
| DWITH_LAPACK= | =ON | |
| - | Enable Trilinos ML functionality | require libraries |
| DWITH_ML=ON | | |
| - | Documentation of the source code | require doxygen and graphviz |
| DWITH_DOC=OF | F | |
| | Revert result file format if ON is | |
| DOLD_RES_FORM | specifical FF | |

The list of variables that can be set with cmake can be confirmed with the following command.

$\$ cmake -L

Other options are as follows.

| Options | Contents | Remarks |
|----------------------------|-------------------------------------|---------------------------------------|
| -DBLA_VENDOR= | Specify vendor name of BLAS and | Refer to the FindBLAS.cmake |
| | LAPACK | |
| _ | Directly specifies BLAS library | Absolute path |
| DBLAS_LIBRARIES= | | |
| - | Directly specifies LAPACK library | Absolute path |
| DLAPACK_LIBRARIES | = | |
| _ | Specify installing path. Default is | If specifies - |
| DCMAKE INSTALL PRESEXLOCAL | | DCMAKE_INSTALL_PREFIX=\$HOME/local,bi |
| | | will copy to \$HOME/local/bin |
| - | Specify C compiler | -DCMAKE_C_COMPILER=icc (ex. |
| DCMAKE_C_COMPILI | ER= | Intel C compiler) |
| - | Specify C++ compiler | -DCMAKE_CXX_COMPILER=icpc |
| DCMAKE_CXX_COME | PILER= | (ex. Intel C++ compiler) |
| - | Specify Fortran compiler | - - |
| DCMAKE_Fortran_COM | MPILER= | DCMAKE_Fortran_COMPILER=ifort |
| | | (ex. Intel Fortran compiler) |
| - | Specify path of libraries | - - |
| DCMAKE_PREFIX_PA | TH= | DCMAKE_PREFIX_PATH=\$HOME/tools |

1.7 About test

This software includes test scripts for validating compiled binaries.

In order to execute the test you need to install ruby in advance. If ruby is already installed, test is automatically enabled.

Test is executed as follows.

```
$ make test
```

Results as follows.

```
Running tests...
```

```
        Test project /home/fistr/FrontISTR/build

        Start 1: Static_exA_Test
        1/23 Test #1: Static_exA_Test
        Passed 3.54 sec

        Start 2: Static_exB_Test
        2/23 Test #2: Static_exB_Test
        Passed 2.51 sec
```

You can output verbosed messages as follow.

```
$ make test ARGS="-VV -j4 -O test_log.txt"
```

Results will output in test_log.txt file. For more information;

```
$ ctest --help
```

1.8 About documentation of source code

For learning or investigating the source code, you can generate HTML documents that describes relationship functions from the source codes.

You need install doxygen and graphviz in advance.

Generated HTML can browse like as follow.

\$ firefox doc/html/index.html

1.9 Enable Debugging

To enable debugging, specify the following option.

```
\ cmake -DCMAKE BUILD TYPE="DEBUG" ...
```

To perform more advanced debugging, specifying the following options is useful for investigating memory leaks.

```
$ cmake -DCMAKE BUILD TYPE="DEBUG" -DDEBUG EXTRA=ON ...
```

1.10 Compile with editing Makefile.conf manually

1.10.1 Editing Makefile.conf

Create Makefile.conf by editing Makefile.conf.org in \${FSTRBUILDDIR} to match the computer environment where this software is to be installed. There are a large number of variables that can be defined, but most of them can be used "as is" (without having to change the default values). For most environments, there should be no need to change variables other than those shown below.

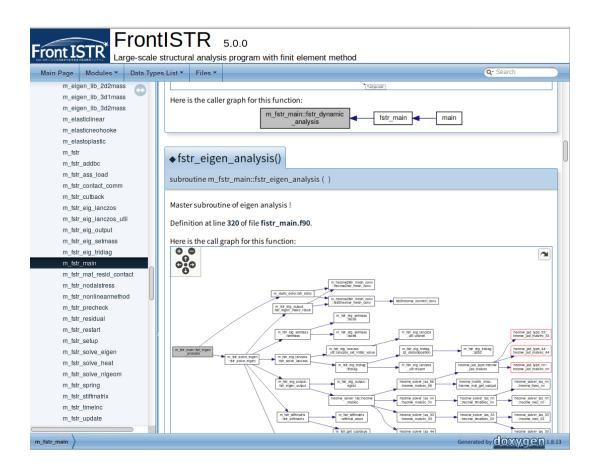


Figure 1: Doxygen

| Variable | Description |
|-------------|---|
| MPIDIR | Specifies the directory where MPI has been installed |
| PREFIX | Specifies the directory where the executable module of this software is to be installed |
| METISDIR | Specifies the directory where METIS has been installed |
| PARMETISDIR | Specifies the directory where ParMETIS has been installed |
| REFINERDIR | Specifies the directory where REVOCAP_Refiner has been installed |
| REVOCAPDIR | Specifies the directory where REVOCAP_Coupler has been installed |
| MUMPSDIR | Specifies the directory where MUMPS has been installed |
| CC | Specifies the C compiler start command |
| CPP | Specifies the C++ compiler start command |
| F90 | Specifies the Fortran 90 compiler start command |

Refer to Appendix A, "List of Makefile.conf Variables" for details on all variables. Refer also to Appendix B, "Makefile.conf Setting Example" for an example of Makefile.conf settings.

1.10.2 Executing setup.sh

Create Makefile by executing the setup.sh shell script in \${FSTRBUILDDIR}, as below.

\$./setup.sh

To generate a library for parallel computing, for example, execute setup.sh with the following options specified.

1.10.2.1 Options specified when setup.sh is executed

| Option | Description | Remarks |
|-----------------|--|--|
| -g or -debug | Generates a library for debugging | |
| -p or -parallel | Generates a library for parallel execution | |
| -with-tools | Generates a tool such as a partitioner | |
| -with-refiner | Includes REVOCAP Refiner | |
| -with-revocap | Includes REVOCAP Coupler | |
| -with-metis | Uses METIS | |
| -with-parmetis | Uses ParMETIS | Disabled at present |
| -with-mkl | Uses Intel MKL | • |
| -with-mumps | Uses MUMPS | |
| -with-lapack | Uses Lapack | Needed for condition number estimation |
| -with-ml | Uses ML | |
| -old-res-format | Revert result file format | |

Examples of setup.sh execution are shown below.

${\bf 1.10.2.2} \quad {\bf Compiling \ for \ parallel \ partitioner}$

If this software is used in parallel execution environment where MPI has installed, execute setup.sh with the -p or --parallel option specified, as below.

\$./setup.sh -p

1.10.2.3 Generating a tool such as a partitioner

If a processing or post-processing tool such as a partitioner (RCB) or visualizer is required, execute setup.sh with the --with-tools option specified, as below.

 $\ ./setup.sh -p --with-tools$

1.10.2.4 Using METIS

If METIS is used with a partitioner in an environment where METIS has been installed, execute setup.sh with the --with-metis option specified, as below.

\$./setup.sh -p ---with-tools ---with-metis

1.10.2.5 Compiling for contact analysis

If this software is used in a sequential processing with contact analysis, execute setup.sh with the —with—mkl or —with—mumps option specified, as below.

Sequential processing

\$./setup.sh --with-mkl

or

\$./setup.sh --with-mumps

If this software is used in a parallel processing with contact analysis, execute setup.sh with -p, --with-metis and --with-mumps options specified, as below.

1.10.3 Executing make

Execute make in \${FSTRBUILDDIR} as below.

\$ make $2 > \& 1 \mid$ tee make.log

It may take sevral minutes to execute make, depending on the computer environment. If an error occurs during execution, take appropriate actions such as reviewing the Makefile.conf

1.10.4 Executing make install

After make has finished executing normally, execute make install to install this software in the directory specified in Makefile.conf, as below.

\$ make install

1.10.5 Installing in Windows environments

In Windows environments, the following UNIX-like environments can be used to install this software according to the above procedures.

• Sequential processing version : MinGW, Cygwin

- Parallel processing version : MinGW + Microsoft MPI, Cygwin + OpenMPI

1.11 Appendix

1.11.1 List of Makefile.conf Variables

1.11.1.1 Setting related to MPI

| Variable name | Description | Default |
|---------------|--|---------|
| MPIDIR | This variable specifies the path to the directory where MPI has been installed. If an MPI compatible compiler automatically refers to the path, there is no need to set this variable together with the following variables. | None |
| MPIBINDIR | This variable specifies the path to the directory where MPI executable files have been installed. | None |
| MPIINCDIR | This variable specifies the path to the directory where MPI header files have been installed. | • |
| MPILIBDIR | This variable specifies the path to the directory where MPI libraries have been installed. | |
| MPILIBS | This variable specifies the MPI library that will be linked to C and Fortran90 object files. | None |

1.11.1.2 Setting related to the installation directory

| Variable name | Description | Default |
|---------------|--|--------------------|
| PREFIX | This variable specifies the path to the directory where this software is to be installed. | \$(HOME)/FrontISTF |
| BINDIR | This variable specifies the path to the directory where the executable files of this software are to be installed. | (PREFIX)/bin |
| INCLUDEDIR | This variable specifies the path to the directory where the header files of this software are to be installed. Normally, there is no need to change the value of this variable from the default value. | \$(PREFIX)/include |
| LIBDIR | This variable specifies the path to the directory where the libraries of this software are to be installed. Normally, there is no need to change the value of this variable from the default value. | \$(PREFIX)/lib |

1.11.1.3 Settings related to METIS

| Variable name | Description | Default |
|---------------|--|----------------------|
| METISDIR | This variable specifies the path to the directory where METIS has been installed. | \$(HOME)/metis |
| METISINCDIR | This variable specifies the path to the directory where the header files (such as metis.h) of METIS have been installed. Normally, there is no need to change the value of this variable from the default value. | \$(METISDIR)/include |
| METISLIBDIR | This variable specifies the path to the directory where the library (libmetis.a) of METIS has been installed. Normally, ther is no need to change the value of this variable from the default value. | (METISDIR)/lib |

1.11.1.4 Settings related to ParMETIS

| Variable name | Description | Default |
|----------------|--|-------------------------|
| PARMETISDIR | This variable specifies the path to the directory where ParMETIS has been installed. | \$(HOME)/ParMetis |
| PAEMETISINCDIR | This variable specifies the path to the directory where the header files (such as parmetis.h) of ParMETIS have been installed. Normally, there is no need to change the value of this variable from the default value. | \$(PARMETISDIR)/include |

| Variable name | Description | Default |
|----------------|---|---------------------|
| PARMETISLIBDIR | This variable specifies the path to the directory where the library (libparmetis.a) of ParMETIS has been installed. Normally, there is no need to change the value of this variable from the default value. | \$(PARMETISDIR)/lib |

${\bf 1.11.1.5} \quad {\bf Settings} \ {\bf related} \ {\bf to} \ {\bf REVOCAP_Refiner}$

| Variable name | Description | Default |
|---------------|---|-------------------------|
| REFINERDIR | This variable specifies the path to the directory where | \$(HOME)/REVOCAP_Refine |
| | REVOCAP_Refiner has been installed. | |
| REFINERINCDIR | This variable specifies the path to the directory where | \$(PARMETISDIR)/include |
| | REVOCAP_Refiner header files have been installed. | |
| | Normally, there is no need to change the value of this | |
| | variable from the default value. | |
| REFINERLIBDIR | This variable specifies the path to the directory where | \$(PARMETISDIR)/lib |
| | REVOCAP_Refiner libraries have been installed. | |
| | Normally, there is no need to change the value of this | |
| | variable from the default value. | |

$1.11.1.6 \quad \textbf{Settings related to REVOCAP_Coupler}$

| Variable name | Description | Default |
|---------------|---|-------------------------|
| REVOCAPDIR | This variable specifies the path to the directory where | \$(HOME)/REVOCAP_Couple |
| | REVOCAP_Coupler has been installed. | |
| REVOCAPINCDIR | This variable specifies the path to the directory where | \$(REVOCAPDIR)/include |
| | REVOCAP_Coupler header files have been installed. | , |
| | Normally, there is no need to change the value of this | |
| | variable from the default value. | |
| REVOCAPLIBDIR | This variable specifies the path to the directory where | \$(REVOCAPDIR)/lib |
| | REVOCAP_Coupler libraries have been installed. | ` |
| | Normally, there is no need to change the value of this | |
| | variable from the default value. | |

1.11.1.7 Settings related to MUMPS

| Variable name | Description | Default |
|---------------|---|------------------|
| MUMPSDIR | This variable specifies the path to the directory where MUMPS has been installed. | \$(HOME)/MUMPS |
| MUMPSINCDIR | This variable specifies the path to the directory where MUMPS header files have been installed. Normally, there is no need to change the value of this variable from the default value. | MUMPSDIR/include |
| MUMPSLIBDIR | This variable specifies the path to the directory where MUMPS libraries have been installed. Normally, there is no need to change the value of this variable from the default value. | \$(MUMPSDIR)/lib |

1.11.1.8 Settins related to ML

| Variable name | Description | Default |
|---------------|--|-------------------|
| MLDIR | This variable specifies the path to the directory where ML is installed. | \$(HOME)/trilinos |
| MLINCDIR | This variable specivies the path to the directory where ML header files are installed. Normally, there is no need to change the value of this variable from the default value. | MLDIR/include |
| MLLIBDIR | This variable specivies the path to the directory where ML libraries are installed. Normally, there is no need to change the value of this variable from the default value. | \$(MLDIR)/lib |

1.11.1.9 Settings related to the C compiler

| Variable name | Description | Default |
|--------------------------|---|----------------|
| $\overline{\mathrm{CC}}$ | This variable specifies the C compiler start command | mpicc |
| CFLAGS | This variable specifies the option to be assigned to the C | |
| | compiler. Normally, there is no need to change the value of | |
| | this variable from the default value. | |
| LDFLAGS | This variable specifies the option to be assigned to the C | $-\mathrm{lm}$ |
| | linker. Normally, there is no need to change the value of | |
| | this variable from the default value. However, when | |
| | REVOCAP_Refiner (written in C++) is to be used and C | |
| | compiler is used for linking C programs, C++ standard | |
| | library (e.glstdc++) needs to be specified here. | |
| OPTFLAGS | This variable specifies the optimization option (or another | -O3 |
| | option) to be assigned to the C compiler. | |
| CLINKER | This variable specifies the linker command for C program. | (CC) |
| | This is used when, for example, REVOCAP_Refiner | |
| | (written in C++) is to be used and C++ compiler needs to | |
| | be used for linking C programs with C++ libraries. | |

1.11.1.10 Settings related to the C++ compiler

| Variable name | Description | Default |
|-----------------|---|---|
| CPP CPPFLAGS | This variable specifies the C++ compiler start command. This variable specifies the option to be assigned to the C++ compiler. Normally, there is no need to change the value of this variable from the default value. However, if Boost Libraries are not automatically referenced from the C++ compiler, use the -I option to specify the directory | mpic++ -DMPICH_IGNORE_CXX_SEEK (Note: This is required for Intel compilers.) |
| CPPLDFLAGS | that contains the include files. This variable specifies the option to be assigned to the C++ linker. Normally, there is no need to change the value of this variable from the default value. | None |
| CPPOPTFLAGS | This variable specifies the optimization option (or another option) to be assigned to the C++ compiler. | -O3 |

${\bf 1.11.1.11} \quad {\bf Settings \ related \ to \ Fortran 90 \ compiler}$

| Variable name | Description | Default |
|---------------|--|---------|
| F90 | This variable specifies the Fortran90 compiler start | mpif90 |
| | command. | |

| Variable name | Description | Default |
|---------------|---|-------------------------|
| F90FLAGS | This variable specifies the option to be assigned to the Fortran90 compiler. Normally, there is no need to change the value of this variable from the default value. | -DMPICH_IGNORE_CXX_SEEK |
| F90LDFLAGS | This variable specifies the option to be assigned to the Fortran90 linker. Normally, there is no need to change the value of this variable from the default value. However, if Intel MKL is used, specify its link option. Also, when REVOCAP_Refiner (written in C++) is to be used and Fortran90 compiler is used for linking Fortran90 programs, C++ standard library (e.glstdc++) needs to be specified here. | None |
| F90OPTFLAGS | This variable specifies the optimization option (or another option) to be assigned to the Fortran90 compiler. | -O2 |
| F90LINKER | This variable specifies the linker command for Fortran90 program. This is used when, for example, REVOCAP_Refiner (written in C++) is to be used and C++ compiler needs to be used for linking Fortran90 programs with C++ libraries. (E.g. on K-computer, "mpiFCCpx -linkfortran" needs to be specified.) | \$(F90) |

${\bf 1.11.1.12} \quad {\bf Settings \ related \ to \ UNIX \ commands}$

| Variable name | Description | Default |
|---------------|--|----------|
| MAKE | This variable specifies the make start command. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | make |
| AR | This variable specifies the command for creating or changing an archive file. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | ar ruv |
| CP | This variable specifies the command for copying files or directories. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | cp -f |
| RM | This variable specifies the command for deleting files or directories. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | rm -f |
| MKDIR | This variable specifies the command for creating directories. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | mkdir —p |
| MV | This variable specifies the command for moving files or directories. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | mv |

1.11.2 Example of Makefile.conf

 $\# \ \mathrm{MPI}$

MPIDIR =

 ${\rm MPIBINDIR} \, = \,$

 $\mathrm{MPILIBDIR} \, = \,$

```
MPIINCDIR =
MPILIBS
# for install option only
           = $(HOME)/FrontISTR
PREFIX
BINDIR
           = $(PREFIX)/bin
LIBDIR
           = \$(PREFIX)/lib
INCLUDEDIR = \$(PREFIX)/include
# Metis
METISDIR
            = $ (HOME) / Metis -4.0
METISLIBDIR = \$(METISDIR)
METISINCDIR = \frac{(METISDIR)}{Lib}
# ParMetis
PARMETISDIR
                = $ (HOME) / ParMetis -3.1
PARMETISLIBDIR = \$(PARMETISDIR)
PARMETISINCDIR = $(PARMETISDIR)/ParMETISLib
# Refiner
REFINERDIR
              = $ (HOME) / REVOCAP_Refiner -1.1.0
REFINERINCDIR = $(REFINERDIR)/Refiner
REFINERLIBDIR = $(REFINERDIR)/lib/x86_64-linux
# Coupler
REVOCAPDIR
              = $(HOME)/REVOCAP Coupler-1.6.2
REVOCAPINCDIR = \$(REVOCAPDIR) / librcap
REVOCAPLIBDIR = \$(REVOCAPDIR) / librcap
# MUMPS
MUMPSDIR
            = $ (HOME) /MUMPS 4.10.0
MUMPSINCDIR = \frac{MUMPSDIR}{include}
MUMPSLIBDIR = MUMPSDIR / 1 i b
\# ML
         = $ (HOME) / trilinos /11.8.1 / ml
MLDIR.
MLINCDIR = $(MLDIR)/include
MLLIBDIR = (MLDIR)/lib
# C compiler settings
         = mpiicc
CC
CFLAGS
LDFLAGS = -lm
OPTFLAGS = -O3
CLINKER = mpiicc
# C++ compiler settings
CPP
            = mpiicpc
            = -DMPICH IGNORE CXX SEEK -I$ (HOME) / include
CPPFLAGS
CPPLDFLAGS
CPPOPTFLAGS = -O3
# Fortran compiler settings
F90
            = mpiifort
F90FLAGS
F90LDFLAGS = -lmkl intel lp64 -lmkl intel thread -lmkl core -liomp5
F90OPTFLAGS = -O2
F90LINKER
           = mpiifort
```

1.11.3 Notes on K-computer and Fujitsu FX10

This version includes tuned codes for K-computer and Fujitsu FX10. However, in order to maximize the performance, a part of the source code needs to be changed for corresponding environment.

File to be changed:

hecmw1/src/solver/solver_33/hecmw_tuning_fx.f90

Changes:

Set the value of parameter TotalSectorCacheSize defined in the file to

- 12 on K-computer,
- 24 on FX10.

Initially, the parameter is set for K-computer.

1.12 Appendix

1.12.1 List of Makefile.conf Variables

1.12.1.1 Setting related to MPI

| Variable name | Description | Default |
|---------------|--|---------|
| MPIDIR | This variable specifies the path to the directory where MPI has been installed. If an MPI compatible compiler automatically refers to the path, there is no need to set this variable together with the following variables. | None |
| MPIBINDIR | This variable specifies the path to the directory where MPI executable files have been installed. | None |
| MPIINCDIR | This variable specifies the path to the directory where MPI header files have been installed. | |
| MPILIBDIR | This variable specifies the path to the directory where MPI libraries have been installed. | ٠ |
| MPILIBS | This variable specifies the MPI library that will be linked to C and Fortran90 object files. | None |

1.12.1.2 Setting related to the installation directory

| Variable name | Description | Default |
|---------------|--|--------------------|
| PREFIX | This variable specifies the path to the directory where this software is to be installed. | \$(HOME)/FrontISTR |
| BINDIR | This variable specifies the path to the directory where the executable files of this software are to be installed. | (PREFIX)/bin |
| INCLUDEDIR | This variable specifies the path to the directory where the header files of this software are to be installed. Normally, there is no need to change the value of this variable from the default value. | \$(PREFIX)/include |
| LIBDIR | This variable specifies the path to the directory where the libraries of this software are to be installed. Normally, there is no need to change the value of this variable from the default value. | \$(PREFIX)/lib |

1.12.1.3 Settings related to METIS

| Variable name | Description | Default |
|---------------|---|----------------|
| METISDIR | This variable specifies the path to the directory where METIS has | \$(HOME)/metis |
| | been installed. | |

| Variable name | Description | Default |
|---------------|--|----------------------|
| METISINCDIR | This variable specifies the path to the directory where the header files (such as metis.h) of METIS have been installed. Normally, there is no need to change the value of this variable from the default value. | \$(METISDIR)/include |
| METISLIBDIR | This variable specifies the path to the directory where the library (librarian) of METIS has been installed. Normally, ther is no need to change the value of this variable from the default value. | \$(METISDIR)/lib |

1.12.1.4 Settings related to ParMETIS

| Variable name | Description | Default |
|----------------|--|---------------------------|
| PARMETISDIR | This variable specifies the path to the directory where | \$(HOME)/ParMetis |
| | ParMETIS has been installed. | |
| PAEMETISINCDIR | This variable specifies the path to the directory where the | $\P(PARMETISDIR)/include$ |
| | header files (such as parmetis.h) of ParMETIS have been | |
| | installed. Normally, there is no need to change the value of | |
| | this variable from the default value. | |
| PARMETISLIBDIR | This variable specifies the path to the directory where the | \$(PARMETISDIR)/lib |
| | library (libparmetis.a) of ParMETIS has been installed. | |
| | Normally, there is no need to change the value of this | |
| | variable from the default value. | |

1.12.1.5 Settings related to REVOCAP_Refiner

| Variable name | Description | Default |
|---------------|---|-------------------------|
| REFINERDIR | This variable specifies the path to the directory where | \$(HOME)/REVOCAP_Refine |
| | REVOCAP_Refiner has been installed. | |
| REFINERINCDIR | This variable specifies the path to the directory where | \$(PARMETISDIR)/include |
| | REVOCAP_Refiner header files have been installed. | |
| | Normally, there is no need to change the value of this | |
| | variable from the default value. | |
| REFINERLIBDIR | This variable specifies the path to the directory where | \$(PARMETISDIR)/lib |
| | REVOCAP_Refiner libraries have been installed. | |
| | Normally, there is no need to change the value of this | |
| | variable from the default value. | |

1.12.1.6 Settings related to REVOCAP_Coupler

| Variable name | Description | Default |
|---------------|---|-------------------------|
| REVOCAPDIR | This variable specifies the path to the directory where | \$(HOME)/REVOCAP_Couple |
| | REVOCAP_Coupler has been installed. | |
| REVOCAPINCDIR | This variable specifies the path to the directory where | \$(REVOCAPDIR)/include |
| | REVOCAP_Coupler header files have been installed. | |
| | Normally, there is no need to change the value of this | |
| | variable from the default value. | |
| REVOCAPLIBDIR | This variable specifies the path to the directory where | \$(REVOCAPDIR)/lib |
| | REVOCAP_Coupler libraries have been installed. | |
| | Normally, there is no need to change the value of this | |
| | variable from the default value. | |

1.12.1.7 Settings related to MUMPS

| Variable name | Description | Default |
|---------------|---|----------------------|
| MUMPSDIR | This variable specifies the path to the directory where MUMPS has been installed. | \$(HOME)/MUMPS |
| MUMPSINCDIR | This variable specifies the path to the directory where MUMPS header files have been installed. Normally, there is no need to change the value of this variable from the default value. | \$(MUMPSDIR)/include |
| MUMPSLIBDIR | This variable specifies the path to the directory where MUMPS libraries have been installed. Normally, there is no need to change the value of this variable from the default value. | \$(MUMPSDIR)/lib |

1.12.1.8 Settins related to ML

| Variable name | Description | Default |
|---------------|--|-------------------|
| MLDIR | This variable specifies the path to the directory where ML is installed. | \$(HOME)/trilinos |
| MLINCDIR | This variable specivies the path to the directory where ML header files are installed. Normally, there is no need to change the value of this variable from the default value. | \$(MLDIR)/include |
| MLLIBDIR | This variable specivies the path to the directory where ML libraries are installed. Normally, there is no need to change the value of this variable from the default value. | \$(MLDIR)/lib |

1.12.1.9 Settings related to the C compiler

| Variable name | Description | Default |
|------------------------|---|----------------|
| $\overline{\text{CC}}$ | This variable specifies the C compiler start command | mpicc |
| CFLAGS | This variable specifies the option to be assigned to the C | |
| | compiler. Normally, there is no need to change the value of | |
| | this variable from the default value. | |
| LDFLAGS | This variable specifies the option to be assigned to the C | $-\mathrm{lm}$ |
| | linker. Normally, there is no need to change the value of | |
| | this variable from the default value. However, when | |
| | REVOCAP_Refiner (written in C++) is to be used and C | |
| | compiler is used for linking C programs, C++ standard | |
| | library (e.glstdc++) needs to be specified here. | |
| OPTFLAGS | This variable specifies the optimization option (or another | -O3 |
| | option) to be assigned to the C compiler. | |
| CLINKER | This variable specifies the linker command for C program. | \$(CC) |
| | This is used when, for example, REVOCAP_Refiner | |
| | (written in C++) is to be used and C++ compiler needs to | |
| | be used for linking C programs with C++ libraries. | |

1.12.1.10 Settings related to the C++ compiler

| Variable name | Description | Default |
|---------------|---|---------|
| CPP | This variable specifies the C++ compiler start command. | mpic++ |

| Variable name | Description | Default |
|---------------|--|---|
| CPPFLAGS | This variable specifies the option to be assigned to the C++ compiler. Normally, there is no need to change the value of this variable from the default value. However, if | -DMPICH_IGNORE_CXX_SEER (Note: This is required for Intel compilers.) |
| | Boost Libraries are not automatically referenced from the C++ compiler, use the -I option to specify the directory that contains the include files. | • / |
| CPPLDFLAGS | This variable specifies the option to be assigned to the C++ linker. Normally, there is no need to change the value of this variable from the default value. | None |
| CPPOPTFLAGS | This variable specifies the optimization option (or another option) to be assigned to the C++ compiler. | -O3 |

1.12.1.11 Settings related to Fortran90 compiler

| Variable name | Description | Default |
|---------------|---|------------------------|
| F90 | This variable specifies the Fortran90 compiler start command. | mpif90 |
| F90FLAGS | This variable specifies the option to be assigned to the Fortran90 compiler. Normally, there is no need to change the value of this variable from the default value. | -DMPICH_IGNORE_CXX_SEE |
| F90LDFLAGS | This variable specifies the option to be assigned to the Fortran90 linker. Normally, there is no need to change the value of this variable from the default value. However, if Intel MKL is used, specify its link option. Also, when REVOCAP_Refiner (written in C++) is to be used and Fortran90 compiler is used for linking Fortran90 programs, C++ standard library (e.glstdc++) needs to be specified here. | None |
| F90OPTFLAGS | This variable specifies the optimization option (or another option) to be assigned to the Fortran90 compiler. | -O2 |
| F90LINKER | This variable specifies the linker command for Fortran90 program. This is used when, for example, REVOCAP_Refiner (written in C++) is to be used and C++ compiler needs to be used for linking Fortran90 programs with C++ libraries. (E.g. on K-computer, "mpiFCCpx -linkfortran" needs to be specified.) | \$(F90) |

1.12.1.12 Settings related to UNIX commands

| Variable name | Description | Default |
|---------------|--|---------|
| MAKE | This variable specifies the make start command. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | make |
| AR | This variable specifies the command for creating or changing an archive file. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | ar ruv |
| СР | This variable specifies the command for copying files or directories. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | cp-f |

| Variable name | Description | Default |
|---------------|---|----------|
| RM | This variable specifies the command for deleting files or directories. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | rm -f |
| MKDIR | This variable specifies the command for creating directories. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | mkdir —p |
| MV | This variable specifies the command for moving files or directories. If options are required, specify them together. Normally, there is no need to change the value of this variable from the default value. | mv |

1.12.2 Example of Makefile.conf

```
# MPI
MPIDIR
MPIBINDIR =
MPILIBDIR =
MPIINCDIR =
MPILIBS
# for install option only
            = $(HOME)/FrontISTR
PREFIX
BINDIR
            = $(PREFIX)/bin
LIBDIR
             = \$(PREFIX)/lib
INCLUDEDIR = \$(PREFIX)/include
# Metis
METISDIR
              = $ (HOME) / Metis -4.0
METISLIBDIR = \$(METISDIR)
METISINCDIR = \frac{METISDIR}{Lib}
# ParMetis
PARMETISDIR
                 = $ (HOME) / ParMetis -3.1
PARMETISLIBDIR = \$(PARMETISDIR)
PARMETISINCDIR = \$(PARMETISDIR)/ParMETISLib
# Refiner
                = $ (HOME) / REVOCAP_Refiner -1.1.0
REFINERDIR
REFINERINCDIR = \$(REFINERDIR) / Refiner
REFINERLIBDIR = $(REFINERDIR)/lib/x86_64-linux
# Coupler
REVOCAPDIR
                = $ (HOME) / REVOCAP Coupler -1.6.2
REVOCAPINCDIR = \$(REVOCAPDIR) / librcap
REVOCAPLIBDIR = \$(REVOCAPDIR) / librcap
# MUMPS
              = $ (HOME) /MUMPS_4.10.0
MUMPSDIR
MUMPSINCDIR = \frac{MUMPSDIR}{include}
\label{eq:mumpsdir} \text{MUMPSDIR} \, = \, \$ \, (\text{MUMPSDIR}) \, / \, \text{li} \, \text{b}
\# \ \mathrm{ML}
          = $ (HOME) / trilinos /11.8.1 / ml
MLINCDIR = \frac{MLDIR}{include}
```

```
MLLIBDIR = \frac{MLDIR}{lib}
# C compiler settings
CC
         = mpiicc
CFLAGS
LDFLAGS = -lm
OPTFLAGS = -O3
CLINKER = mpiicc
# C++ compiler settings
            = mpiicpc
CPPFLAGS
            = -DMPICH_IGNORE_CXX_SEEK -I$ (HOME) / include
CPPLDFLAGS
CPPOPTFLAGS = -O3
# Fortran compiler settings
F90
            = mpiifort
F90FLAGS
F90LDFLAGS = -lmkl_intel_lp64 -lmkl_intel_thread -lmkl_core -liomp5
F90OPTFLAGS = -O2
F90LINKER
            = mpiifort
```

1.12.3 Notes on K-computer and Fujitsu FX10

This version includes tuned codes for K-computer and Fujitsu FX10. However, in order to maximize the performance, a part of the source code needs to be changed for corresponding environment.

File to be changed:

hecmw1/src/solver/solver_33/hecmw_tuning_fx.f90

Changes:

Set the value of parameter TotalSectorCacheSize defined in the file to

- 12 on K-computer,
- 24 on FX10.

Initially, the parameter is set for K-computer.

1.13 Appendix: Example of installation procedure to CentOS7.6(cmake)

We will explain how to install this software and how to build external libraries required this software on CentOS7.6. More information for building each libraries, refer to their installation manuals.

1.13.1 Preparation

At first, install the basic build toolchains and libraries as follows.

```
$ su
# yum group mark install "Development Tools"
# yum update
# yum install openmpi-devel cmake
# exit
```

Configure the MPI environment settings as follows.

```
$ module purge
$ module local mpi/openmpi-x86_64
```

If you write the above two lines in \$HOME/.bash_profile, the settings will be reflected even after the next login.

Please check compilers and compiler wrappers for MPI works propery as follows.

```
$ which gcc g++ gfortran mpicc mpic++ mpifort
/usr/bin/gcc
/usr/bin/g++
/usr/bin/gfortran
/usr/lib64/openmpi/bin/mpicc
/usr/lib64/openmpi/bin/mpic++
/usr/lib64/openmpi/bin/mpifort
```

1.13.2 Installing libraries

Compile and install required libraries this software. Working directory is \$HOME/work, destination directory for install is \$HOME/local.

And add \$HOME/local/bin to PATH environment variable as follows.

```
$ cd $HOME
$ mkdir work
$ mkdir -p local/bin local/lib local/include
$ export PATH=$HOME/local/bin:$PATH
```

1.13.2.1 Downloads

Downloads the following software and save it to working directory \$HOME/work.

| Software | Link |
|----------------------------------|---|
| REVOCAP_Refiner-1.1.04.tar.gz | https://www.frontistr.com/ |
| FrontISTR_V50.tar.gz | http://www.frontistr.com/ |
| OpenBLAS-0.2.20.tar.gz | http://www.openblas.net/ |
| metis-5.1.0.tar.gz | http://glaros.dtc.umn.edu/gkhome/metis/metis/download |
| scalapack-2.0.2.tgz | http://www.netlib.org/scalapack/ |
| $MUMPS_5.1.2.tar.gz$ | http://mumps.enseeiht.fr/ |
| trilinos-12.14.1-Source.tar.bz 2 | https://trilinos.org/download/ |

1.13.2.2 Compiling REVOCAP_Refiner

```
$ cd $HOME/work
$ tar xvf REVOCAP_Refiner-1.1.04.tar.gz
$ cd REVOCAP_Refiner-1.1.04
$ make
$ cp lib/x86_64-linux/libRcapRefiner.a $HOME/local/lib
$ cp Refiner/rcapRefiner.h $HOME/local/include
```

1.13.2.3 Compiling OpenBLAS

```
$ cd $HOME/work
$ tar xvf OpenBLAS-0.2.20.tar.gz
$ make BINARY=64 NO_SHARED=1 USE_OPENMP=1
$ make PREFIX=$HOME/local install
```

1.13.2.4 Compiling METIS

\$ cd \$HOME/work

```
  \text{star xvf metis} -5.1.0. tar.gz 
\ cd metis -5.1.0
$ make config prefix=~/local cc=gcc openmp=1
$ make
$ make install
1.13.2.5 Compiling ScaLAPACK
$ cd $HOME/work
 tar xvf scalapack -2.0.2.tgz 
d cd scalapack -2.0.2
$ mkdir build
\ cmake -DCMAKE_INSTALL_PREFIX=$HOME/local \
        -DCMAKE_EXE_LINKER_FLAGS="-fopenmp"
        -DCMAKE_BUILD_TYPE="Release" \
        -DBLAS LIBRARIES-$HOME/local/lib/libopenblas.a \
        -DLAPACK_LIBRARIES=$HOME/local/lib/libopenblas.a \
$ make
$ make install
1.13.2.6 Compiling MUMPS
$ cd $HOME/work
tar xvf MUMPS_5.1.2.tar.gz
$ cp Make.inc/Makefile.inc.generic Makefile.inc
Change the following parts of copied Makefile.inc.
$ vi Makefile.inc
$ cp Make.inc/Makefile.inc.generic Makefile.inc
$ vi Makefile.inc
LMETISDIR = \frac{(HOME)}{local}
IMETIS
          = -I$ (LMETISDIR) / include
LMETIS
          = -L\$(LMETISDIR)/lib -lmetis
ORDERINGSF = -Dmetis -Dpord
CC
        = mpicc
FC
        = mpifort
FL
        = mpifort
LAPACK = -L\$(HOME)/local/lib -lopenblas
SCALAP = -L\$(HOME)/local/lib -lscalapack
INCPAR = -I/usr/include/openmpi-x86 64
LIBPAR = \frac{SCALAP}{-L/usr/lib64/openmpi/lib -lmpi}
LIBBLAS = -L\$(HOME)/local/lib -lopenblas
        = -O -DBLR_MT -fopenmp
OPTF
OPTC
        = -O -I. -fopenmp
OPTL
        = -O -fopenmp
```

Then execute make.

```
$ make
$ cp lib/*.a $HOME/local/lib
$ cp include /*.h $HOME/local/include
1.13.2.7 Compiling Trilinos ML
 cd $HOME/work
  tar xvf trilinos -12.14.1 - Source.tar.gz
 cd trilinos -12.14.1-Source
$ mkdir build
$ cmake -DCMAKE_INSTALL_PREFIX=$HOME/local \
        -DCMAKE C COMPILER=mpicc \
        -DCMAKE_CXX_COMPILER=mpic++
        -DCMAKE_Fortran_COMPILER=mpifort \
        -DTPL_ENABLE_MP⊨ON \
        -DTPL ENABLE LAPACK=ON \
        -DTPL_ENABLE_SCALAPACK=ON \
        -DTPL_ENABLE_METIS=ON \
        -DTPL ENABLE MUMPS-ON \
        -DTPL_MUMPS_INCLUDE_DIRS=$HOME/local/include \
        -DTrilinos\_ENABLE\_ML=ON \setminus
        -DTrilinos_ENABLE_Zoltan=ON \
        -DTrilinos ENABLE OpenMP=ON \
        -DTrilinos ENABLE Amesos=ON \
        -DTrilinos_ENABLE_ALL_OPTIONAL_PACKAGES=OFF \
        -DBLAS_LIBRARY_DIRS=$HOME/local/lib \
        -DLAPACK_LIBRARY_DIRS=$HOME/local/lib"
        -DSCALAPACK_LIBRARY_DIRS=$HOME/local/lib"
        -DBLAS LIBRARY NAMES="openblas"
        -DLAPACK LIBRARY NAMES="openblas"
        -DSCALAPACK LIBRARY NAMES="scalapack" \
$ make
 make install
1.13.3 Compiling FrontISTR
Finishing compiling above libraries, compile FrontISTR.
$ cd $HOME/work/FrontISTR
$ mkdir build
 cd build
 cmake -DCMAKE_INSTALL_PREFIX=$HOME/FrontISTR \
        -DWITH_ML=ON \
        -DBLAS_LIBRARIES=$HOME/local/lib/libopenblas.a \
        -DLAPACK LIBRARIES-$HOME/local/lib/libopenblas.a \
1.13.3.1 Executing make
```

Execute make command.

\$ make

When execute make simultaneously, specify option -j.

make - i4

Reduce compile time when increase the number of simultaneous.

1.13.3.2 Executing make install

```
$ make install
```

. . .

FrontISTR will be installed to \$(HOME)/FrontISTR/bin.

1.13.3.3 Testing FrontISTR

```
Run sample case in the tutorial directory and check running of FrontISTR.
```

```
$ cd $HOME/work/FrontISTR/tutorial
$ cd 01_elastic_hinge
$ $HOME/FrontISTR/bin/fistr1
 Step control not defined! Using default step=1
 fstr_setup: OK
 Start visualize PSF 1 at timestep 0
 loading step=
                  1
 sub\_step=1,
                current_time= 0.0000E+00, time_inc= 0.1000E+01
 loading_factor=
                     0.0000000
                                 1.0000000
### 3x3 BLOCK CG, SSOR, 1
      1
           1.903375E+00
      2
           1.974378E+00
      3
           2.534627E\!\!+\!\!00
      4
           3.004045E+00
      5
           3.202633E+00
      6
           3.203864E+00
```

When finished analysis, displayed message as follows.

2969 iterations 9.391687E-09set-up time 4.108060E-01solver time 6.506822E+01solver/comm time : 4.342469E-01solver/matvec 1.923199E+01solver/precond : 2.688405E+01solver/1 iter 2.191587E-02: work ratio (%)9.933263E+01

Start visualize PSF 1 at timestep 1 ### FSTR_SOLVE_NLGEOM FINISHED!

| TOTAL TIME | (sec) | : | 74.93 |
|------------|-------|---|-------|
| | (sec) | | 1.86 |
| solve | (sec) | : | 73.07 |

FrontISTR Completed !!

1.14 Appendix: Example of installation procedure to CentOS7.6 (Makefile.conf)

We will explain how to install this software and how to build external libraries required this software on CentOS7.6. More information for building each libraries, refer to their installation manuals.

1.14.1 Preparation

At first, install the basic build toolchains and libraries as follows.

```
$ su
# yum group mark install "Development Tools"
# yum update
# yum install openmpi-devel cmake
# exit
```

Configure the MPI environment settings as follows.

```
$ module purge
$ module local mpi/openmpi-x86_64
```

If you write the above two lines in \$HOME/.bash_profile, the settings will be reflected even after the next login.

Please check compilers and compiler wrapper for MPI works properly as follow.

```
$ which gcc g++ gfortran mpicc mpic++ mpifort
/usr/bin/gcc
/usr/bin/g++
/usr/bin/gfortran
/usr/lib64/openmpi/bin/mpicc
/usr/lib64/openmpi/bin/mpic++
/usr/lib64/openmpi/bin/mpifort
```

1.14.2 Installing libraries

Compile and install required libraries this software. Working directory is \$HOME/work, destination directory for install is \$HOME/local.

And add \$HOME/local/bin to PATH environment variable as follows.

```
$ cd $HOME
$ mkdir work
$ mkdir -p local/bin local/lib local/include
$ export PATH=$HOME/local/bin:$PATH
```

1.14.2.1 Downloads

Downloads the following software and save it to working directory \$HOME/work.

| Software | Link |
|----------------------------------|---|
| REVOCAP_Refiner-1.1.04.tar.gz | https://www.frontistr.com/ |
| $FrontISTR_V50.tar.gz$ | https://www.frontistr.com/ |
| OpenBLAS-0.2.20.tar.gz | http://www.openblas.net/ |
| metis-5.1.0.tar.gz | http://glaros.dtc.umn.edu/gkhome/metis/metis/download |
| scalapack-2.0.2.tgz | http://www.netlib.org/scalapack/ |
| $MUMPS_5.1.2.tar.gz$ | http://mumps.enseeiht.fr/ |
| trilinos-12.14.1-Source.tar.bz 2 | https://trilinos.org/download/ |

```
1.14.2.2 Compiling REVOCAP_Refiner
```

```
$ cd $HOME/work
$ tar xvf REVOCAP_Refiner-1.1.04.tar.gz
$ cd REVOCAP_Refiner-1.1.04
$ make
$ cp lib/x86_64-linux/libRcapRefiner.a $HOME/local/lib
$ cp Refiner/rcapRefiner.h $HOME/local/include
```

1.14.2.3 Compiling OpenBLAS

```
$ cd $HOME/work
$ tar xvf OpenBLAS-0.2.20.tar.gz
$ make BINARY=64 NO_SHARED=1 USE_OPENMP=1
$ make PREFIX=$HOME/local install
```

1.14.2.4 Compiling METIS

```
$ cd $HOME/work
$ tar xvf metis -5.1.0.tar.gz
$ cd metis -5.1.0
$ make config prefix=$HOME/local cc=gcc openmp=1
$ make
$ make install
```

1.14.2.5 Compiling ScaLAPACK

1.14.2.6 Compiling MUMPS

```
$ cd $HOME/work
$ tar xvf MUMPS_5.1.2.tar.gz
$ cd MUMPS_5.1.2
$ cp Make.inc/Makefile.inc.generic Makefile.inc
Change the following parts of copied Makefile.inc
$ vi Makefile.inc
$ cp Make.inc/Makefile.inc.generic Makefile.inc
$ vi Makefile.inc
$ vi Makefile.inc
LMETISDIR = $ (HOME)/local
IMETIS = -I$ (LMETISDIR)/include
LMETIS = -L$ (LMETISDIR)/lib -lmetis
```

ORDERINGSF = -Dmetis -Dpord

```
CC
        = mpicc -fopenmp
FC
        = mpifort -fopenmp
        = mpifort -fopenmp
FL
LAPACK = -L\$(HOME)/local/lib -lopenblas
SCALAP = -L\$(HOME)/local/lib -lscalapack
INCPAR = -I/usr/include/openmpi-x86\_64
LIBPAR = \frac{SCALAP}{-L/usr/lib64/openmpi/lib-lmpi}
LIBBLAS = -L\$(HOME)/local/lib -lopenblas
OPTF
        = -O -DBLR MT -fopenmp
OPTC
        = -O -I. -fopenmp
OPTL
        = -O -fopenmp
Then execute make.
$ make
$ cp lib/*.a $HOME/local/lib
$ cp include /*.h $HOME/local/include
1.14.2.7 Compiling Trilinos ML
$ cd $HOME/work
  tar xvf trilinos -12.14.1-Source.tar.gz
delta cd trilinos -12.14.1-Source
$ mkdir build
-DCMAKE C COMPILER=mpicc \
        -DCMAKE_CXX_COMPILER=mpic++ \
        -DCMAKE_Fortran_COMPILER=mpifort \
        -DTPL_ENABLE_MP⊫ON \
        -DTPL ENABLE LAPACK=ON \
        -DTPL_ENABLE_SCALAPACK=ON \
        -DTPL ENABLE METIS=ON \
        -DTPL_ENABLE_MUMPS=ON \
        -DTPL MUMPS INCLUDE DIRS-$HOME/local/include \
        -DTrilinos\_ENABLE\_ML=ON \setminus
        -DTrilinos\_ENABLE\_Zoltan=ON \setminus
        -DTrilinos_ENABLE_OpenMP=ON \
        -DTrilinos\_ENABLE\_Amesos=ON \setminus
        -DTrilinos_ENABLE_ALL_OPTIONAL_PACKAGES=OFF \
        -DBLAS LIBRARY DIRS-$HOME/local/lib \
        -DLAPACK LIBRARY DIRS-$HOME/local/lib" \
        -DSCALAPACK LIBRARY DIRS=$HOME/local/lib" \
        -DBLAS_LIBRARY_NAMES="openblas" \
        -DLAPACK_LIBRARY_NAMES="openblas"
        -DSCALAPACK LIBRARY NAMES="scalapack" \
$ make
 make install
```

1.14.3 Compiling FrontISTR

Finishing compiling above libraries, compile FrontISTR.

```
$ cd $HOME/work
 tar xvf FrontISTR_V50.tar.gz
$ cd FrontISTR
```

MKLINCDIR = (MKLDIR) / include

1.14.3.1 Editing Makefile.conf

```
Copy template as Makefile.conf.org to Makfile.conf. Then edit Makefile.conf as follows.
$ cp Makefile.conf.org Makefile.conf
  vi Makefile.conf
#
#
#
                                                 #
      Setup Configulation File for FrontISTR
#
                                                 #
# MPI
MPIDIR
               =/usr/lib64/openmpi
              = $ (MPIDIR) / bin
MPIBINDIR
               = $(MPIDIR)/lib
MPILIBDIR
MPIINCDIR
               =/usr/include/openmpi-x86_64
MPILIBS
               = -lmpi - lmpi _cxx - lmpi _mpifh
# for install option only
PREFIX
              = $ (HOME) / FrontISTR
BINDIR
               = \$(PREFIX)/bin
LIBDIR.
              = \$(PREFIX)/lib
INCLUDEDIR
              = $(PREFIX)/include
# Metis
METISDIR
               = \$(HOME)/local
METISLIBDIR
               = $(METISDIR)/lib
               = $(METISDIR)/include
METISINCDIR
HECMW_METIS_VER = 5
# ParMetis
PARMETISDIR
               = $ (HOME) / local
PARMETISLIBDIR = \$(PARMETISDIR) / 1ib
PARMETISINCDIR = $(PARMETISDIR)/include
# Refiner
              = $ (HOME) / local
REFINERDIR
REFINERINCDIR = \$(REFINERDIR)/include
REFINERLIBDIR = (REFINERDIR)/lib
# Coupler
REVOCAPDIR
               = \$(HOME) / local
REVOCAPINCDIR = \$(REVOCAPDIR) / include
REVOCAPLIBDIR = \$(REVOCAPDIR) / 1ib
# MUMPS
MUMPSDIR
               = \$(HOME)/local
MUMPSINCDIR
               = $ (MUMPSDIR) / include
MUMPSLIBDIR
               = $ (MUMPSDIR) / lib
MUMPSLIBS
               = -ldmumps -lmumps_common -lpord -L$HOME/local/lib -lscalapack
# MKL PARDISO
MKLDIR
           = \$ (HOME) /
```

```
\# ML
MLDIR.
               = \$(HOME)/local
               = $(MLDIR)/include
MLINCDIR
MLLIBDIR
               = $ (MLDIR) / lib
               = -lml -lamesos -ltrilinosss -lzoltan -lepetra -lteuchosremainder -lteuchosnu
MLLIBS
# C compiler settings
CC
               = mpicc -fopenmp
CFLAGS
LDFLAGS
               = -lstdc++-lm
OPTFLAGS
               = -O3
# C++ compiler settings
CPP
               = mpic++-fopenmp
CPPFLAGS
CPPLDFLAGS
CPPOPTFLAGS
               = -O3
# Fortran compiler settings
F90
               = mpif90 - fopenmp
F90FLAGS
F90LDFLAGS
               = -lstdc++ -L\$(HOME)/local/lib -lopenblas
F90OPTFLAGS
               = -O2
               =-cpp
F90FPP
F90LINKER
               = mpif90 -fopenmp
MAKE
                = make
AR
                = ar ruv
MV
                = mv - f
CP
               = cp - f
               = \ rm \ -f
RM
```

1.14.3.2 Executing setup.sh

MKLLIBDIR = (MKLDIR) / lib

Finished to edit Makefile.conf, then execute setup.sh.

= mkdir -p

1.14.3.3 Executing make

Execute make command.

\$ make

MKDIR

1.14.3.4 Executing make install

\$ make install

FrontISTR will be installed to \$(HOME)/FrontISTR/bin.

1.14.3.5 Testing FrontISTR

Run sample case in the tutorial directory and check running of FrontISTR.

```
$ cd $HOME/work/FrontISTR/tutorial
$ cd 01_elastic_hinge
$ $HOME/FrontISTR/bin/fistr1
 Step control not defined! Using default step=1
 fstr_setup: OK
 Start visualize PSF 1 at timestep 0
 loading step=
                                 0.0000E+00, time_inc=
 sub\_step=1,
                                                         0.1000E+01
                 current_time=
 loading_factor=
                     0.0000000
                                  1.0000000
### 3x3 BLOCK CG, SSOR, 1
      1
            1.903375E+00
      2
            1.974378E+00
      3
            2.534627E+00
            3.004045E+00
      4
      5
            3.202633E+00
      6
            3.203864E+00
. . .
. . .
When finished analysis, displayed message as follows.
   2966
            1.143085E-08
   2967
            1.078272E-08
   2968
            1.004759E-08
   2969
            9.372882E-09
### Relative residual = 9.39169E-09
### summary of linear solver
      2969 iterations
                             9.391687E-09
    set-up time
                             4.108060E-01
    solver time
                             6.506822E+01
    solver/comm time :
                             4.342469E-01
    solver/matvec
                             1.923199E+01
    solver/precond
                             2.688405E+01
    solver/1 iter
                             2.191587E-02
    work ratio (%)
                             9.933263E+01
 Start visualize PSF 1 at timestep 1
### FSTR_SOLVE_NLGEOM FINISHED!
    TOTAL TIME (sec) :
                             74.93
            pre (sec):
                              1.86
          solve (sec):
                             73.07
```

FrontISTR Completed !!

1.15 Appendix: Example of installation procedure to Ubuntu18.04(cmake)

We will explain how to install this software and how to build external libraries required this software on Ubuntu18.04. More information for building each libraries, refer to their installation manuals.

1.15.1 Preparation

At first, install the basic build toolchains and libraries as follows.

\$ sudo apt install build-essential gfortran cmake openmpi-bin libopenmpi-dev

Please check compilers and compiler wrappers for MPI works propery.

```
$ which gcc g++ gfortran mpicc mpic++ mpifort
/usr/bin/gcc
/usr/bin/g++
/usr/bin/gfortran
/usr/bin/mpicc
/usr/bin/mpic++
/usr/bin/mpifort
```

1.15.2 Installing libraries

Compile and install required libraries this software. Working directory is \$HOME/work, destination directory for install is \$HOME/local.

And add \$HOME/local/bin to PATH environment variable as follows.

- \$ cd \$HOME
- \$ mkdir work
- \$ mkdir -p local/bin local/lib local/include
- \$ export PATH=\$HOME/local/bin:\$PATH

1.15.2.1 Downloads

Downloads the following software and save it to working directory \$HOME/work.

| Software | Link |
|----------------------------------|---|
| REVOCAP_Refiner-1.1.04.tar.gz | https://www.frontistr.com/ |
| $FrontISTR_V50.tar.gz$ | https://www.frontistr.com/ |
| OpenBLAS-0.2.20.tar.gz | http://www.openblas.net/ |
| metis-5.1.0.tar.gz | http://glaros.dtc.umn.edu/gkhome/metis/metis/download |
| scalapack-2.0.2.tgz | http://www.netlib.org/scalapack/ |
| $MUMPS_5.1.2.tar.gz$ | http://mumps.enseeiht.fr/ |
| trilinos-12.14.1-Source.tar.bz 2 | https://trilinos.org/download/ |

1.15.2.2 Compiling REVOCAP_Refiner

```
$ cd $HOME/work
$ tar xvf REVOCAP_Refiner-1.1.04.tar.gz
$ cd REVOCAP_Refiner-1.1.04
$ make
$ cp lib/x86_64-linux/libRcapRefiner.a $HOME/local/lib
$ cp Refiner/rcapRefiner.h $HOME/local/include
```

1.15.2.3 Compiling OpenBLAS

```
$ cd $HOME/work
$ tar xvf OpenBLAS-0.2.20.tar.gz
$ make BINARY=64 NO_SHARED=1 USE_OPENMP=1
$ make PREFIX=$HOME/local install
```

```
1.15.2.4 Compiling METIS
$ cd $HOME/work
$ tar xvf metis -5.1.0.tar.gz
delta cd metis -5.1.0
$ make config prefix=$HOME/local cc=gcc openmp=1
$ make
$ make install
1.15.2.5 Compiling ScaLAPACK
$ cd $HOME/work
 $ tar xvf scalapack -2.0.2.tgz 
\ cd scalapack -2.0.2
$ mkdir build
-DCMAKE_EXE_LINKER_FLAGS="-fopenmp" \
        -DBLAS LIBRARIES-$HOME/local/lib/libopenblas.a \
        -DLAPACK LIBRARIES-$HOME/local/lib/libopenblas.a \
$ make
$ make install
1.15.2.6 Compiling MUMPS
$ cd $HOME/work
 tar xvf MUMPS 5.1.2.tar.gz
\ cd MUMPS 5.1.2
$ cp Make.inc/Makefile.inc.generic Makefile.inc
Change the following parts of copied Makefile.inc.
$ vi Makefile.inc
$ cp Make.inc/Makefile.inc.generic Makefile.inc
$ vi Makefile.inc
LMETISDIR = \$(HOME) / local
          = -I$ (LMETISDIR) / include
IMETIS
LMETIS
          = -L\$(LMETISDIR)/lib -lmetis
ORDERINGSF = -Dmetis - Dpord
CC
        = mpicc -fopenmp
FC
        = mpifort -fopenmp
FL
        = mpifort -fopenmp
LAPACK = -L\$(HOME)/local/lib -lopenblas
SCALAP = -L\$(HOME)/local/lib -lscalapack
INCPAR =
LIBPAR = \$(SCALAP)
LIBBLAS = -L\$(HOME)/local/lib -lopenblas
Then execute make.
$ make
$ cp lib/*.a $HOME/local/lib
```

\$ cp include/*.h \$HOME/local/include

1.15.2.7 Compiling Trilinos ML

```
$ cd $HOME/work
 tar \ xvf \ trilinos -12.14.1 - Source.tar.gz
 cd trilinos -12.14.1-Source
 mkdir build
 cmake -DCMAKE_INSTALL_PREFIX=$HOME/local \
        -DCMAKE C COMPILER=mpicc \
        -DCMAKE CXX COMPILER=mpic++ \
        -DCMAKE Fortran COMPILER=mpifort \
        -DTPL ENABLE MP⊨ON \
        -DTPL ENABLE LAPACK=ON \
        -DTPL_ENABLE_SCALAPACK=ON \
        −DTPL_ENABLE_METIS=ON \
        -DTPL ENABLE MUMPS-ON
        -DTrilinos ENABLE ML=ON
        -DTrilinos_ENABLE_Zoltan=ON
        -DTrilinos_ENABLE_OpenMP=ON \
        -DTrilinos ENABLE Amesos=ON \
        -DTrilinos ENABLE ALL OPTIONAL PACKAGES=OFF \
        -DBLAS_LIBRARY_DIRS=$HOME/local/lib \
        -DLAPACK_LIBRARY_DIRS=$HOME/local/lib"
        -DSCALAPACK LIBRARY DIRS=$HOME/local/lib" \
        -DBLAS LIBRARY NAMES="openblas"
        -DLAPACK_LIBRARY_NAMES="openblas"
        -DSCALAPACK_LIBRARY_NAMES="scalapack" \
$ make
$ make install
```

1.15.3 Compiling FrontISTR

Finishing compiling above libraeies, compile FrontISTR.

1.15.3.1 Executing make

\$ make

When execute make simultaneously, specify option -j.

make - j4

Reduce compile time when increase the number of simultaneous.

1.15.3.2 Executing make install

\$ make install

FrontISTR will be installed to \$(HOME)/FrontISTR/bin.

1.15.3.3 Testing FrontISTR

```
Run sample case in the tutorial directory and check running of FrontISTR.
$ cd $HOME/work/FrontISTR/tutorial
$ cd 01_elastic_hinge
$ $HOME/FrontISTR/bin/fistr1
 Step control not defined! Using default step=1
 fstr setup: OK
 Start visualize PSF 1 at timestep 0
 loading step=
 sub\_step=1,
                 current_time=
                                 0.0000E+00, time_inc= 0.1000E+01
                     0.0000000
                                  1.0000000
 loading factor=
### 3x3 BLOCK CG, SSOR, 1
            1.903375E+00
      1
      2
            1.974378E+00
      3
            2.534627E+00
      4
            3.004045E+00
      5
            3.202633E+00
      6
            3.203864E+00
```

When finished analysis, displayed message as follows.

. . .

```
2966
            1.143085E-08
            1.078272\mathrm{E}{-08}
   2967
   2968
            1.004759E-08
   2969
            9.372882E-09
### Relative residual = 9.39169E-09
### summary of linear solver
      2969 iterations
                             9.391687E-09
    set-up time
                             4.108060E-01
                     :
    solver time
                             6.506822E+01
    solver/comm time :
                             4.342469E-01
    solver/matvec
                             1.923199E+01
    solver/precond
                             2.688405E+01
    solver/1 iter
                             2.191587E-02
    work ratio (%)
                             9.933263E+01
```

Start visualize PSF 1 at timestep 1 ### FSTR_SOLVE_NLGEOM FINISHED!

| TOTAL TIME | (sec) | : | 74.93 |
|------------|-------|---|-------|
| pre | (sec) | : | 1.86 |
| solve | (sec) | : | 73.07 |
| | | | |

FrontISTR Completed !!

1.16 Appendix: Example of installation procedure to Ubuntu18.04(Makefile.conf)

We will explain how to install this software and how to build external libraries required this software on Ubuntu18.04. More information for building each libraries, refer to their installation manuals.

1.16.1 Preparation

At first, install the basic build toolchains and libraries as follows.

\$ sudo apt install build-essential gfortran cmake openmpi-bin libopenmpi-dev

Please check compilers and compiler wrappers for MPI works propery.

```
$ which gcc g++ gfortran mpicc mpic++ mpifort
/usr/bin/gcc
/usr/bin/g++
/usr/bin/gfortran
/usr/bin/mpicc
/usr/bin/mpic++
/usr/bin/mpifort
```

1.16.2 Installing libraries

Compile and install required libraries this software. Working directory is \$HOME/work, destination directory for install is \$HOME/local.

And add \$HOME/local/bin to PATH environment variable as follows.

```
$ cd $HOME
```

- \$ mkdir work
- \$ mkdir -p local/bin local/lib local/include
- \$ export PATH=\$HOME/local/bin:\$PATH

1.16.2.1 Downloads

Downloads the following software and save it to working directory \$HOME/work.

| Software | Link |
|----------------------------------|---|
| REVOCAP_Refiner-1.1.04.tar.gz | https://www.frontistr.com/ |
| $FrontISTR_V50.tar.gz$ | https://www.frontistr.com/ |
| OpenBLAS-0.2.20.tar.gz | http://www.openblas.net/ |
| metis-5.1.0.tar.gz | http://glaros.dtc.umn.edu/gkhome/metis/metis/download |
| scalapack-2.0.2.tgz | http://www.netlib.org/scalapack/ |
| $MUMPS_5.1.2.tar.gz$ | http://mumps.enseeiht.fr/ |
| trilinos-12.14.1-Source.tar.bz 2 | https://trilinos.org/download/ |

1.16.2.2 Compiling REVOCAP_Refiner

```
$ cd $HOME/work
$ tar xvf REVOCAP_Refiner-1.1.04.tar.gz
$ cd REVOCAP_Refiner-1.1.04
$ make
$ cp lib/x86_64-linux/libRcapRefiner.a $HOME/local/lib
$ cp Refiner/rcapRefiner.h $HOME/local/include
```

1.16.2.3 Compiling OpenBLAS

```
$ cd $HOME/work
$ tar xvf OpenBLAS-0.2.20.tar.gz
$ make BINARY=64 NO_SHARED=1 USE_OPENMP=1
$ make PREFIX=$HOME/local install
```

```
1.16.2.4 Compiling METIS
 $ cd $HOME/work
     tar xvf metis -5.1.0.tar.gz
 delta delt
 $ make config prefix=$HOME/local cc=gcc openmp=1
 $ make
 $ make install
1.16.2.5 Compiling ScaLAPACK
 $ cd $HOME/work
   tar xvf scalapack -2.0.2.tgz 
 \ cd scalapack -2.0.2
 $ mkdir build
 \ cmake <code>-DCMAKE_INSTALL_PREFIX=$HOME/local</code> \
                         -DCMAKE_EXE_LINKER_FLAGS="-fopenmp" \
                         -DWITH ML=ON \
                         -DBLAS LIBRARIES-$HOME/local/lib/libopenblas.a \
                         -DLAPACK_LIBRARIES=$HOME/local/lib/libopenblas.a \
 $ make
 $ make install
1.16.2.6 Compiling MUMPS
 $ cd $HOME/work
 $ tar xvf MUMPS 5.1.2.tar.gz
 $ cd MUMPS 5.1.2
 $ cp Make.inc/Makefile.inc.generic Makefile.inc
Change the following parts of copied Makefile.inc.
 $ vi Makefile.inc
 $ cp Make.inc/Makefile.inc.generic Makefile.inc
 $ vi Makefile.inc
LMETISDIR = \frac{(HOME)}{local}
IMETIS
                              = -I$ (LMETISDIR) / include
                              = -L\$(LMETISDIR)/lib -lmetis
LMETIS
ORDERINGSF = -Dmetis - Dpord
CC
                        = mpicc
FC
                        = mpifort
FL
                        = mpifort
LAPACK = -L\$(HOME)/local/lib -lopenblas
SCALAP = -L\$(HOME)/local/lib -lscalapack
INCPAR =
LIBPAR = \$(SCALAP)
LIBBLAS = -L\$(HOME)/local/lib -lopenblas
```

OPTF

OPTC OPTL = -O -DBLR_ML -fopenmp = -O -I. -fopenmp

= -O -fopenmp

```
Then execute make.
```

```
$ make
$ cp lib/*.a $HOME/local/lib
$ cp include/*.h $HOME/local/include
```

1.16.2.7 Compiling Trilinos ML

```
cd $HOME/work
 tar xvf trilinos -12.14.1 - Source.tar.gz
delta cd trilinos -12.14.1-Source
$ mkdir build
$ cmake -DCMAKE INSTALL PREFIX=$HOME/local \
        -DCMAKE_C_COMPILER=mpicc \
        -DCMAKE_CXX_COMPILER=mpic++ \
        -DCMAKE Fortran COMPILER=mpifort \
        -DTPL_ENABLE_MP⊨ON \
        -DTPL_ENABLE_LAPACK=ON \
        -DTPL_ENABLE_SCALAPACK=ON \
        -DTPL ENABLE METIS=ON \
        -DTPL_ENABLE_MUMPS=ON
        −DTrilinos ENABLE ML=ON \
        -DTrilinos ENABLE Zoltan=ON \
        -DTrilinos_ENABLE_OpenMP=ON
        -DTrilinos\_ENABLE\_Amesos=ON \setminus
        -DTrilinos_ENABLE_ALL_OPTIONAL_PACKAGES=OFF \
        -DBLAS LIBRARY DIRS-$HOME/local/lib \
        -DLAPACK_LIBRARY_DIRS=$HOME/local/lib" \
        -DSCALAPACK_LIBRARY_DIRS=$HOME/local/lib" \
        -DBLAS_LIBRARY_NAMES="openblas" \
        -DLAPACK_LIBRARY_NAMES="openblas"
        -DSCALAPACK_LIBRARY_NAMES="scalapack" \
$ make
$ make install
```

1.16.3 Compiling FrontISTR

Finishing compiling above libraries, compile FrontISTR.

```
$ cd $HOME/work
$ tar xvf FrontISTR_V50.tar.gz
$ cd FrontISTR
```

1.16.3.1 Edit Makefile.conf

Copy template as Makefile.conf.org to Makefile.conf. Then edit Makefile.conf as follows.

```
MPIBINDIR
                = /usr/bin
MPILIBDIR
               = $(MPIDIR)/lib
               = $(MPIDIR)/include
MPIINCDIR
MPILIBS
               = -lmpi - lmpi cxx - lmpi mpifh
# for install option only
PREFIX
               = $ (HOME) / FrontISTR
BINDIR
               = $(PREFIX)/bin
LIBDIR
               = \$(PREFIX)/lib
INCLUDEDIR
               = $(PREFIX)/include
# Metis
METISDIR
                = \$(HOME) / local
                = $(METISDIR)/lib
METISLIBDIR
               = $(METISDIR)/include
METISINCDIR
HECMW_METIS_VER = 5
# ParMetis
PARMETISDIR
                = $ (HOME) / local
PARMETISLIBDIR = $(PARMETISDIR) / lib
PARMETISINCDIR = $(PARMETISDIR)/include
# Refiner
                = \$(HOME) / local
REFINERDIR
REFINERINCDIR = $(REFINERDIR)/include
REFINERLIBDIR = \$(REFINERDIR) / lib
# Coupler
REVOCAPDIR
                = \$(HOME) / local
REVOCAPINCDIR = \$(REVOCAPDIR) / include
REVOCAPLIBDIR = \$(REVOCAPDIR) / lib
# MUMPS
                = \$(HOME) / local
MUMPSDIR
MUMPSINCDIR
               = $ (MUMPSDIR) / include
               = $ (MUMPSDIR) / lib
MUMPSLIBDIR
MUMPSLIBS
                = -ldmumps -lmumps common -lpord -L$(HOME)/local/lib -lscalapack
# MKL PARDISO
           = \$ (HOME) /
MKLDIR
MKLINCDIR = \$(MKLDIR)/include
MKLLIBDIR = (MKLDIR) / lib
# ML
                = \$(HOME) / local
MLDIR
                = $(MLDIR)/include
MLINCDIR
               = $ (MLDIR) / lib
MLLIBDIR
               = -lml -lamesos -ltrilinosss -lzoltan -lepetra -lteuchosremainder -lteuchosnu
MLLIBS
# C compiler settings
CC
                = mpicc -fopenmp
CFLAGS
LDFLAGS
               = -lstdc++-lm
OPTFLAGS
                = -O3
# C++ compiler settings
                = mpic++-fopenmp
CPPFLAGS
```

CPPLDFLAGS

```
CPPOPTFLAGS = -O3
```

```
# Fortran compiler settings
F90
                = mpif90 -fopenmp
F90FLAGS
                = -lstdc++ -L\$(HOME)/local/lib -lopenblas
F90LDFLAGS
F90OPTFLAGS
                = -O2
F90FPP
                = -cpp
F90LINKER
                = mpif90 - fopenmp
MAKE
                = make
AR
                = ar ruv
MV
                = mv - f
CP
                = cp - f
RM
                = rm - f
MKDIR.
                = mkdir -p
```

1.16.3.2 Executing setup.sh

Finished to edit Makefile.conf, then execute setup.sh.

```
$ ./setup.sh -p --with-tools --with-refiner \
--with-metis --with-mumps --with-lapack --with-ml
```

1.16.3.3 Executing make

Execute make command.

\$ make

. . .

1.16.3.4 Executing make install

\$ make install

FrontISTR will be installed to \$(HOME)/FrontISTR/bin.

1.16.3.5 Testing FrontISTR

Run sample case in the tutorial directory and check running of FrontISTR.

```
$ cd $HOME/work/FrontISTR/tutorial
$ cd 01_elastic_hinge
$ $HOME/FrontISTR/bin/fistr1
 Step control not defined! Using default step=1
 fstr setup: OK
 Start visualize PSF 1 at timestep 0
 loading step=
                  1
 sub\_step=1,
                               0.0000E+00, time inc= 0.1000E+01
                current_time=
                                 1.0000000
 loading_factor=
                    0.0000000
### 3x3 BLOCK CG, SSOR, 1
      1
           1.903375E+00
      2
           1.974378E+00
      3
           2.534627E+00
           3.004045E+00
      4
      5
           3.202633E+00
           3.203864E+00
```

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When finished analysis, displayed message as follows.

```
2966
            1.143085E-08
            1.078272E-08
   2967
            1.004759E-08
   2968
   2969
            9.372882E-09
### Relative residual = 9.39169E-09
### summary of linear solver
      2969 iterations
                            9.391687E-09
    set-up time
                            4.108060E-01
    solver time
                            6.506822E+01
    solver/comm time :
                            4.342469E-01
    solver/matvec
                            1.923199E+01
    solver/precond
                             2.688405E+01
                      :
    solver/1 iter
                            2.191587E-02
                      :
    work ratio (%)
                            9.933263E+01
```

Start visualize PSF 1 at timestep 1 ### FSTR_SOLVE_NLGEOM FINISHED!

| TOTAL TIME | (sec) | : | 74.93 |
|------------|-------|---|-------|
| pre | (sec) | : | 1.86 |
| solve | (sec) | : | 73.07 |

FrontISTR Completed !!

1.17 Appendix: Example of installation procedure to Windows10(Makefile.conf)

We will explain how to install this software and how to build external libraries required this software on Windows10. More information for building each libraries, refer to their installation manuals.

1.17.1 Preparation

At first, install the basic build toolchains and libraries as follows.

1.17.1.1 Installation of compilers and toolchains for Windows

First, install development environment. Development environment uses MSYS2 in this example.

https://www.msys2.org

Download 64bit installer named msys2-x86_64-xxxxxxxx.exe (xxxxxxxx is version number) and install it.

1.17.1.2 Installing binary package

Finished to install above software, run windows command prompt named MSYS2 MinGW 64-bit, then install other required software.

```
(MINGW64) pacman -S base-devel mingw-w64-x86_64-toolchain \ \begin{array}{c} \text{mingw-w64-x86\_64-cmake} \setminus \\ \text{mingw-w64-x86\_64-binutils} \setminus \\ \text{mingw-w64-x86\_64-perl} \setminus \\ \text{git} \end{array}
```

Please check compilers works properly as follows.

```
(MINGW64) which gcc g++ gfortran
/mingw64/bin/gcc
/mingw64/bin/g++
/mingw64/bin/gfortran
```

1.17.2 Installing libraries

Compile and install required libraries this software. Working directory is \$HOME/work, destination directory for install is \$HOME/local.

And add \$HOME/local/bin to PATH environment variable as follows.

```
(MINGW64) cd $HOME
(MINGW64) mkdir work
(MINGW64) mkdir -p local/bin local/lib local/include
(MINGW64) export PATH—$HOME/local/bin:$PATH
```

1.17.2.1 Installing MPI

In this example, MPI libraries and runtime uses Microsoft MPI.

You can download runtime (msmpisetup.exe) and SDK (msmpisdk.msi) from the following URL.

Download Microsoft MPI v10.0

1.17.2.1.1 Generating .a format library file

To link Microsoft MPI with gcc/gfortran provided from MinGW-w64, convert library format from DLL to .a.

```
(MINGW64) cd $HOME/local/lib
(MINGW64) gendef /c/Windows/System32/msmpi.dll
(MINGW64) dlltool -d msmpi.def -l libmsmpi.a -D /c/Windows/System32/msmpi.dll
(MINGW64) ls
libmsmpi.a msmpi.def
```

1.17.2.1.2 Modifying header files provided from MS-MPI

Copy original header files from installation directory to current directory.

1.17.2.2 Downloads

Downloads the following software and save it to working directory \$HOME/work.

| Software | Link |
|---------------------------------|---|
| REVOCAP_Refiner-1.1.04.tar.gz | https://www.frontistr.com/ |
| $FrontISTR_V50.tar.gz$ | https://www.frontistr.com/ |
| OpenBLAS-0.2.20.tar.gz | http://www.openblas.net/ |
| metis-5.1.0.tar.gz | http://glaros.dtc.umn.edu/gkhome/metis/metis/download |
| scalapack-2.0.2.tgz | http://www.netlib.org/scalapack/ |
| $MUMPS_5.1.2.tar.gz$ | http://mumps.enseeiht.fr/ |
| trilinos-12.14.1-Source.tar.bz2 | https://trilinos.org/download/ |

1.17.2.3 Compiling REVOCAP_Refiner

```
(MINGW64) cd $HOME/work

(MINGW64) tar xvf REVOCAP_Refiner-1.1.04.tar.gz

(MINGW64) cd REVOCAP_Refiner-1.1.04

(MINGW64) make

(MINGW64) cp lib/x86_64-linux/libRcapRefiner.a $HOME/local/lib

(MINGW64) cp Refiner/rcapRefiner.h $HOME/local/include
```

1.17.2.4 Installing OpenBLAS

(MINGW64) pacman -S mingw-w64-x86 64-openblas

1.17.2.5 Compiling METIS

```
(MINGW64) cd \frac{HOME}{work}
(MINGW64) tar xvf metis -5.1.0. tar.gz
(MINGW64) cd metis -5.1.0
```

Correct the following file to fit MinGW environment.

- Makefile
- GKlib/gk_arch.h
- GKlib/getopt.c

```
% vim Makefile
line:60 change from
cd $(BUILDDIR) && cmake $(CURDIR) $(CONFIG FLAGS)
cd $(BUILDDIR) && cmake -G "MSYS Makefiles" $(CURDIR) $(CONFIG_FLAGS)
(MINGW64) vim GKlib/gk\_arch.h
line:44 remove
  #include <sys/resource.h>
(MINGW64) vim GKlib/gk getopt.h
line:54 remove following lines
/* Function prototypes */
extern int gk_getopt(int __argc, char **_argv, char *__shortopts);
extern int gk_getopt_long(int __argc, char **__argv, char *__shortopts,
              struct gk_option *__longopts, int *__longind);
extern int gk_getopt_long_only (int __argc, char **_argv,
              char *__shortopts, struct gk_option *__longopts, int *__longind);
(MINGW64) make config prefix=$HOME/local/cc=gcc openmp=1
(MINGW64) make
(MINGW64) make install
```

1.17.2.6 Compiling ScaLAPACK

```
(MINGW64) cd $HOME/work
(MINGW64) tar xvf scalapack -2.0.2.tgz
(MINGW64) cd scalapack -2.0.2
```

Copy template SLmake.inc.example to SLmake.inc. Then edit SLmake.inc as follows.

```
(MINGW64) cp SLmake.inc.example SLmake.inc
(MINGW64) vi SLmake.inc
   The fortran and C compilers, loaders, and their flags
FC
               = gfortran -fno-range-check
CC
               = gcc
NOOPT
               = -00
FCFLAGS
               = -O3 -I\$ (HOME) / local / include
CCFLAGS
               = -O3 -I\$ (HOME) / local / include
FCLOADER
               = \$(FC)
CCLOADER
               = $(CC)
FCLOADFLAGS
               = $(FCFLAGS) -L$(HOME)/local/lib -lmsmpi
               = $(CCFLAGS) -L$(HOME)/local/lib -lmsmpi
CCLOADFLAGS
   BLAS, LAPACK (and possibly other) libraries needed for linking test programs
#
BLASLIB
               = -lopenblas
LAPACKLIB
               = -lopenblas
               = $(LAPACKLIB) $(BLASLIB)
LIBS
(MINGW64) make
(MINGW64) cp libscalapack.a $HOME/local/lib
Finished to make, then copy libray.
Although an error is displayed at the end of compilation, ignore it.
1.17.2.7 Compiling MUMPS
(MINGW64) cd $HOME/work
(MINGW64) tar xvf MUMPS_5.1.2.tar.gz
(MINGW64) cd MUMPS 5.1.2
(MINGW64) cp Make.inc/Makefile.inc.generic Makefile.inc
Change the following parts of copied Makefile.inc.
(MINGW64) vi Makefile.inc
(MINGW64) cp Make.inc/Makefile.inc.generic Makefile.inc
(MINGW64) vi Makefile.inc
LMETISDIR = $(HOME)/local
IMETIS
          = -I$ (LMETISDIR) / include
          = -L\$(LMETISDIR)/lib -lmetis
LMETIS
ORDERINGSF = -Dmetis -Dpord
CC
        = gcc
FC
        = gfortran -fno-range-check
FL
        = gfortran
LAPACK = -lopenblas
SCALAP = -L\$(HOME)/local/lib -lscalapack
INCPAR = -I\$ (HOME) / local / include
```

```
LIBPAR = (SCALAP) (LAPACK) -L(HOME)/local/lib -lmsmpi
LIBBLAS = -lopenblas
LIBOTHERS = -lpthread -fopenmp
Then execute make.
(MINGW64) make
(MINGW64) cp lib/*.a $HOME/local/lib
(MINGW64) cp include /*.h $HOME/local/include
1.17.2.8 Compiling Trilinos ML
(MINGW64) cd $HOME/work
(MINGW64) tar xvf trilinos -12.14.1-Source.tar.gz
(MINGW64) cd trilinos -12.14.1-Source
(MINGW64) mkdir build
(MINGW64) cmake -G "MSYS Makefiles" \
        -DCMAKE INSTALL PREFIX="$HOME/local" \
        -DCMAKE_CXX_FLAGS="-I$HOME/local/include" \
        -DCMAKE_C_FLAGS="-I$HOME/local/include" \
        -DBLAS_LIBRARY_NAMES="openblas" \
        -DLAPACK_LIBRARY_NAMES="openblas"
        -DMPI_USE_COMPILER_WRAPPERS=OFF \
        -DMPI_C_HEADER_DIR="$HOME/local/include" \
        -DMPI CXX HEADER DIR="$HOME/local/include" \
        -DTPL_ENABLE_MP⊨ON \
        -DTrilinos_ENABLE_OpenMP=ON \
        -DTrilinos\_ENABLE\_ML=ON \setminus
        -DTrilinos_ENABLE_Zoltan=ON \
        -DTrilinos_ENABLE_ALL_OPTIONAL_PACKAGES=OFF \
(MINGW64) make
(MINGW64) make install
1.17.3 Compiling FrontISTR
Finishing compiling above libraries, compile FrontISTR.
(MINGW64) cd $HOME/work
(MINGW64) tar xvf FrontISTR_V50.tar.gz
(MINGW64) cd FrontISTR
1.17.3.1 Editing Makefile.conf
Copy template as Makefile.conf.org to Makefile.conf. Then edit Makefile.conf as follows.
(MINGW64) cp Makefile.conf.org Makefile.conf
(MINGW64) vi Makefile.conf
#
                                                #
#
      Setup Configulation File for FrontISTR
                                                 #
#
# MPI
MPIDIR
              = \$(HOME) / local
```

```
= "/c/Program\ Files/Microsoft\ MPI/Bin/"
MPIBINDIR.
MPILIBDIR
               = $(MPIDIR)/lib
               = $(MPIDIR)/include
MPIINCDIR
MPILIBS
               =-lmsmpi
# for install option only
PREFIX
               = $ (HOME) / FrontISTR
BINDIR
               = $(PREFIX)/bin
LIBDIR
               = \$(PREFIX)/lib
INCLUDEDIR
               = $(PREFIX)/include
# Metis
METISDIR
               = \$(HOME) / local
               = $(METISDIR)/lib
METISLIBDIR
METISINCDIR
               = $(METISDIR)/include
HECMW_METIS_VER = 5
# ParMetis
               = \$(HOME)/local
PARMETISDIR
PARMETISLIBDIR = $(PARMETISDIR)/lib
PARMETISINCDIR = $(PARMETISDIR)/include
# Refiner
               = \$(HOME)/local
REFINERDIR
REFINERINCDIR = $(REFINERDIR)/include
REFINERLIBDIR = \frac{(REFINERDIR)}{1ib}
# Coupler
REVOCAPDIR
               = \$(HOME) / local
REVOCAPINCDIR = \$(REVOCAPDIR) / include
REVOCAPLIBDIR = \$(REVOCAPDIR) / lib
# MUMPS
               = \$(HOME) / local
MUMPSDIR
MUMPSINCDIR
               = $ (MUMPSDIR) / include
               = $(MUMPSDIR)/lib
MUMPSLIBDIR
MUMPSLIBS
               = -ldmumps -lmumps common -lpord -L$HOME/local/lib -lscalapack
# MKL PARDISO
           = \$ (HOME) /
MKLDIR
MKLINCDIR = \$(MKLDIR)/include
MKLLIBDIR = (MKLDIR) / lib
# ML
               = \$(HOME) / local
MLDIR
               = $(MLDIR)/include
MLINCDIR
               = $(MLDIR)/lib
MLLIBDIR
               = -lml - lzoltan - lws2 32
MLLIBS
# C compiler settings
CC
               = gcc -fopenmp
               = -D WINDOWS
CFLAGS
               = -lstdc++-lm
LDFLAGS
OPTFLAGS
               = -O3
# C++ compiler settings
               = g++-fopenmp
CPPFLAGS
               = -D WINDOWS
CPPLDFLAGS
```

```
CPPOPTFLAGS = -O3
```

```
# Fortran compiler settings
F90
                = gfortran -fopenmp -fno-range-check
F90FLAGS
F90LDFLAGS
               = -lstdc++-lopenblas
F90OPTFLAGS
                = -O2
F90FPP
                = -cpp
F90LINKER
               = gfortran -fopenmp
MAKE
                = make
AR
                = ar ruv
MV
               = mv - f
CP
                = cp - f
RM
               = rm - f
MKDIR.
                = mkdir -p
```

1.17.3.2 Executing setup.sh

Finished to edit Makefile.conf, then execute setup.sh.

```
(MINGW64) ./setup.sh -p --with-tools --with-refiner \
--with-metis --with-mumps --with-lapack --with-ml
```

1.17.3.3 Executing make

Execute make command.

(MINGW64) make

. . .

1.17.3.4 Executing make install

```
(MINGW64) make install
```

FrontISTR will be installed to \$(HOME)/FrontISTR/bin.

1.17.3.5 Testing FrontISTR

```
Run sample case in the tutorial directory and check running of FrontISTR.
```

```
(MINGW64) cd $HOME/work/FrontISTR/tutorial
(MINGW64) cd 01_elastic_hinge
(MINGW64$) $HOME/FrontISTR/bin/fistr1
 Step control not defined! Using default step=1
 fstr setup: OK
 Start visualize PSF 1 at timestep 0
 loading step=
                  1
 sub\_step=1,
                               0.0000E+00, time inc= 0.1000E+01
                current_time=
                                 1.0000000
 loading_factor=
                    0.0000000
### 3x3 BLOCK CG, SSOR, 1
      1
           1.903375E+00
      2
           1.974378E+00
      3
           2.534627E+00
           3.004045E+00
      4
      5
           3.202633E+00
           3.203864E+00
```

When finished analysis, displayed message as follows.

1.143085E-082966 2967 1.078272E-08 $1.004759\mathrm{E}{-08}$ 2968 2969 9.372882E-09### Relative residual = 9.39169E-09### summary of linear solver 2969 iterations 9.391687E-09 $\operatorname{set}-\operatorname{up}$ time $4.108060\mathrm{E}{-01}$ solver time 6.506822E+01solver/comm time : 4.342469E-01solver/matvec 1.923199E+01solver/precond $2.688405\mathrm{E}{+}01$ solver/1 iter 2.191587E-02work ratio (%) 9.933263E+01

Start visualize PSF 1 at timestep 1 ### FSTR_SOLVE_NLGEOM FINISHED!

| pre (sec) : 1.86 | 93 |
|---------------------|----|
| 1 () 70 0 | 36 |
| solve (sec): 73.0 | 07 |

FrontISTR Completed !!

1.17.3.6 Supplement

To run in an environment where MinGW is not installed, you need to place following files in the same directory as FrontISTR fistr1 .exe.

- libwinpthread-1.dll
- \bullet libgfortran-3.dll
- $\bullet \ \ libgcc_s_seh-1.dll$
- libgomp-1.dll
- libstdc++-6.dll
- $\bullet \quad lib quad math-0.dll$

You can find these libraries from

 $C: \backslash \mingw64 \backslash bin$

You also need to setup Microsoft MPI runtime (MSMpiSetup.exe).