MFIX SIMULATIONS FOR
1 Mega Watt Pilot Device

Installation Guide and User Manual

Version 2015.1.3

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1. INSTALLATION

CCSI 1MW simulations are custom MFIX simulations. For that reason, the general installation procedure in this user manual follows that of MFIX [1]. In this session, only the 1MW specific installation procedure will be covered in details, leaving the general MFIX steps referring to the MFIX manual.

1.1. Prerequisites

The hardware and software prerequisites follow exactly that of MFIX [1].

1.2. Third Party Software

Open-source, multi-platform data analysis and visualization application ParaView is recommended for the MFIX simulation post-processing purpose. Users can download ParaView software online from http://www.paraview.org/.

Users can choose other similar visualization tools (for example, *Visit*) for the post-processing need.

1.3. Product Installation

This session will only describe the steps to build CFD models for 1MW CFD simulations. It is assumed that users have downloaded MFIX source files of version 2014-1, set environment variables and alias, and built `mfix.exe` on their chosen platform under `$InstallDir/mfix/model`. Users can build either a serial version or a parallel version of `mfix.exe` following instructions in [1].

Download file named CCSI_1MWCFD.tgz from the following URL:
https://www.acceleratecarboncapture.org/drupal/product/1mw_cfd

```
Unzip the file, you will get three directories: src, docs, and scripts
The following files are under src directory:
     calc_mu_s.f
     allocate_arrays.f
     check_data
     check_data_30.f
     drag_gs.f
     drag_ss.f
     ic_mod.f
     init_namelist.f
     namelist.inc
     rrates0.f
     set_ic.f
     solve_energy_eq.f
     source_u_s.f
     source_v_s.f
     species.inc
     usr0.f
```

```
usr_init_namelist.f
usr_mod.f
usrnlst.inc
usr_rates.f
```

Note that check_data is a subdirectory containing two files:
```
check_bc_inflow.f
check_initial_conditions.f
```

This Installation Guide/User Manual file CCSI_Software_Install_1MW.docx is available under docs directory.

The script files, which are useful for pre- and post-processing of the 1MW CFD simulations, are under scripts directory:
```
PP1MW.pl
PostMfix.pm
MyMath.pm
Util.pm
```
mfix.dat
mfix.mod
Modify1MW2.pl
RunCase
RunAll.pl
ProcessAll.pl

Build custom code for 1MW system simulations

The 1MW system custom code should be built on top of MFIX official release of September 2014 (Version 2014-1). This release can be downloaded from MFIX web site:
https://mfix.netl.doe.gov/mfix/download-mfix
The installation from the official release should create and populate content under `$InstallDir`, i.e., $HOME/mfix.

Create a directory for 1MW, e.g., `$HOME/CCSI/1MW`, and copy all the custom source code files to the directory. In the 1MW directory type "`sh $InstallDir/model/make_mfix`" and follow instructions on [1] to build the model. The build process will compile object files and generate a custom `mfix.exe` in directory `$InstallDir/mfix/model`. Upon successful compilation, `mfix.exe` is also copied to `$HOME/CCSI/1MW`.

2. SIMULATIONS

A sample model input file `mfix.dat` for the 1MW simulation is included in the scripts directory. Users can choose to run serial or parallel version of the CFD simulation. For more details, please refer to [1] for general MFIX simulations.

The 1MW simulations consist of large number of simulations with 14 varying parameters with values designed by the uncertainty quantification (UQ) analysis. In the following, a brief instruction is provided to summarize the automation procedure that facilitates the simulations and post-processing needs.

2.1. PRE-PROCESSING

For both pre-processing and post-processing, the user should copy the Perl script files to $HOME/*bin* directory that is included in PATH variable:

```
PP1MW.pl
PostMfix.pm
MyMath.pm
Util.pm
```
Modify1MW2.pl
RunAll.pl
ProcessAll.pl

The user should create a run directory (i.e., *$RunDir=$HOME/1MWRuns*) and copy the following files to the run directory:

      mfix.dat
      mfix.mod
      RunCase
      UQ_351_design_32D_1MW.txt

For all Perl script files, the user must check and change the first line to the local Perl setting unless the file starts with
```
#!/usr/bin/env perl
```

Change this line accordingly to the user's Perl script bin directory
```
use lib "/pic/people/kevinlai/bin";
```

For the run script *RunCase*, the user must check and modify the following to conform to the local setting:
1. Linux/Unix bash setting
2. Module loading: make it consistent with the compiler choice
3. email address
4. location of mfix.exe
5. limit on the total run time of the job allocation
6. Command for a parallel run: currently it is "mpirun –np" but the user must check with his/her own Linux system setting.
7. If the number of processors is changed in the model file mfix.dat (i.e., NODESI * NODESJ * NODESK), make sure that the run script is modified to match the new value.
8. If mfix.exe is built serial, make sure NODESI= NODESJ=NODESK=1 in mfix.dat

After the modifications, run the script in *$RunDir:*
./Modify1MW2.pl

This script does the following:
1. Create 351 sub-directories, Case001 to Case351
2. Copy mfix.mod to mfix.dat at each case sub-directory
3. Modify mfix.dat according to the parameter settings defined in *UQ_351_design_32D_1MW.txt*
4. Copy file *RunCase* to *RCasexxx* sub-directory (i.e., *RCase012*)

The user can go to each case sub-directory and run the batch script *RCasexxx*. Alternatively, the user can run all simulations by
./RunAll.pl

2.2. POST-PROCESSING

The user can choose any post-processing tool to analyze the simulation result, e.g., the official MFIX post-mfix script or the open-source ParaView software.

Alternatively, a Perl script PP1MW.pl provided in this product can be used to automated the post-processing. Go to the simulation directory, e.g., *Case012* and run
PP1MW.pl –o result_file

The data in the result file should be self-explanatory. It prints all the QOIs (quantity of interest) for the 1MW system simulations.

3. REFERENCES

[1]   MFIX – Multiphase Flow with Interphase eXchanges, Version MFIX-2014-1. Download available for members: https://mfix.netl.doe.gov/mfix/download-mfix