Manual for Cantera installation and its coupling with OpenFOAM

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1 Introduction

The main objecive of this file is to expalin the installation of Cantera in MSI@UMN step by step and to show the necessary modifications on OpenFOAM to take advantage of the functions in Cantera for usage in OpenFOAM.

2 Cantera installation

1. Cantera installation needs some libraries, such python, numpy et al. Though most of these required libraries have already been installed in MSI, reinstalling them with the recommended versions in Cantera is strongly recommended (to avoid conflict among different library versions . To do this, the recommended way is using conda.

$ module load conda

$ conda create –name cantera python=3 scons cython boost numpy

This command will download and install all the packages to a conda environment called ”cantera”.

$ conda activate cantera

With those commands, an environment called cantera is installed in your machine. To check where is this environment installed, use this command:

$ conda info –envs

The path of the cantera environment installation will be used in the later configuration.

2. Now refer to the Cantera website and follow the instructions of ”compiling Cantera from source“.

Note 1: Before building and installing Cantera, add these code into your cantera.conf file under the root of your cantera src directory:

python3_package = ’full’

boost_inc_dir = ’/path/to/conda/install/folder/envs/cantera/include’

Note 2: the default Cantera installation path have to be changed into the directory where you want to install Cantera. This could be done by:

$ scons build prefix = ’path/to/the/directory/you/want/to/install/Cantera’

3. Cantera is now installed and let us test it. Upload the CanteraDemo folder

into your MSI home directory and change the cantera head file include path and the library path in the Makefile. We can use this command to set up the basic environment before using cantera:

$ source /home/canteraInstall/bin/setup_cantera

Compile the code and run. If everything is fine, you will see the Demo program print information of a 0D autoignition case with the GRI mechanism.

3 OpenFOAM setting to use Cantera

1. Provided that you have already installed OpenFOAM in your machine (MSI), copy and paste everything in the setup_cantera file to /OpenFOAM/etc/bashrc. Note: you can omit the LD_LIBRARY_PATH part when copying and pasting because the libcantera file will be moved into the bin folder in the $WM_PROJECT_USER path.

2. In the OpenFOAM/etc/bashrc file, also remember to define another two envrionment variables for OpenFOAM:

Location of Cantera files

export WM_CANTERA_DIR=/$HOME/$WM_PROJECT/cantera/include

Location of Cantera mechanisms

export CANTERA_DATA=/$HOME/$WM_PROJECT/canteraInstall/share/cantera/data

The first variable will be used when compiling OpenFOAM libraries and solvers with Cantera head files, while the second one is used to specify where you store your chemical mechanisms.

4 Remarks

Now everything is all set and we can start designing codes in OpenFOAM to take advantage of the functions provided in Cantera.