Setting Up ESP/CAPS and MYSTRAN (Modified Nov. 19, 2019)

Steps to get ESP/CAPS to Run:

- 1. Download ESP/CAPS from the following link: https://acdl.mit.edu/ESP/PreBuilts/
- 2. Download ESP116Lin.tgz. Save in the folder of your choice (we have stored it in a folder called ESP).
- 3. tar -xzvf ESP116Lin.tgz
- 4. cd ES116Lin/ESP116
- 5. ./setup.sh {to set up the environment variables in ESPenv.sh}
- 6. Now you need to environment variables. You have two options:
 - 1. Option One
 - 1. cd EngSketchPad
 - 2. source ESPenv.sh {to set environment variables}
 - 3. Do this every time you open a new terminal
 - 2. Option Two
 - 1. Add the following lines to your ~/.bashrc file (see Figure 3)

```
cd ESP/ESP116Lin/ESP116/EngSketchPad source ESPenv.sh cd ~
```

7. You should now be able to run the pyCAPS examples found in EngSketchPad/CAPSexamples/pyCAPS directory.

Steps to get MYSTRAN to Run from pyCAPS:

- 1. Download MYSTRAN for Linux and save the file in the directory where you want it stored (We saved it in MYSTRAN).
- 2. tar -xzvf MYSTRAN_Linux_64.tar.gz
- 3. cd MYSTRAN/MYSTRAN_Linux_64

- 4. ldd mystran.exe
 - 1. If it says the libmkl*.so shared libraries can't be found then install this software too. You have two options:
 - 1. Download these files from the Box folder. It is provided along with this document.
 - 2. Download these files from https://software.intel.com/en-us/mkl/choose-download/linux. You will need to make an account through Intel in order to download the files. Once you have done that, click on "Register and Download" option.
 - store in MYSTRAN folder.
 - tar -xzvf l_mkl_2019.5.281.tgz
 - cd l_mkl_2019.5.281
 - ./install.sh {Follow the prompts to install the software with the default options.}
- 5. The libmkl*.so files need to be accessible from your \$LD_LIBRARY_PATH, so go into the ESPenv.sh file (this is located in the EngSketchPad directory) and add following directories to this file. You should see a line beginning with:

export LD_LIBRARY_PATH=

Add the highlighted portion to the end of this line as shown below.

/home/bcrow/Documents/ESP116Lin/ESP116/Python2.7/lib:/home/bcrow/Documents/ESP116Lin/ESP116/OpenCASCADE-7.3.1/lib:/home/bcrow/Documents/ESP116Lin/ESP116/EngSketchPad/lib:~/intel/compilers_and_libraries/linux/mkl/lib/intel64:~/intel/compilers_and_libraries/linux/lib/intel64

- NOTE: instead of bcrow, it should show your username directory. If the intel folder isn't in your home directory, you will need to modify your path accordingly.

```
gener PATH=../home/bcrow/Documents/ESP116Lin/ESP116/Python2.7/bin:/home/bcrow/Documents/ESP116Lin/ESP116/EngSketchPad/bin:$PATH
export ESP_ARCH-LINUX64
export ESP_ROOT-/home/bcrow/Documents/ESP116Lin/ESP116/DepenCASCADE-7.3.1
export ESP_ROOT-/home/bcrow/Documents/ESP116Lin/ESP116/OpenCASCADE-7.3.1
export CARACH=.
export CARACH=.
export CARACH=.
export PATHONING=/bcrow/Documents/ESP116Lin/ESP116/Python2.7/lib/home/bcrow/Documents/ESP116Lin/ESP116/Python2.7/lib-/home/bcrow/Documents/ESP116Lin/ESP116/Python2.7/lib-/python2.7'
export PATHONING=/bcrow/Documents/ESP116Lin/ESP116/Python2.7/lib-/python2.7'
export PATHONING=/bcrow/Documents/ESP116Lin/ESP116/EngSketchPad/lib
export CAPS_GLYPH=/home/bcrow/Documents/ESP116Lin/ESP116/EngSketchPad/src/CAPS/aim/pointwise/glyph
export CAPS_GLYPH=/home/bcrow/Documents/ESP116Lin/ESP116/EngSketchPad/src/CAPS/aim/pointwise/glyph
export SLUGS_START="firefox /home/bcrow/Documents/ESP116Lin/ESP116/EngSketchPad/SluGs/Slugs.html"
export SLUGS_START="firefox /home/bcrow/Documents/ESP116Lin/ESP116/EngSketchPad/SluGs/Slugs.html"
export ESP_START="firefox /home/bcrow/Documents/ESP116Lin/ESP116/EngSketchPad/Src/CAPS/CAPS/viewer/capsViewer.html"
export ESP_START="firefox /home/bcrow/Documents/ESP116Lin/ESP116/EngSketchPad/Src/CAPS/CAPS/viewer/capsViewer.html"
export ESP_START="firefox /home/bcrow/Documents/ESP116Lin/ESP116/EngSketchPad/wvCllent/wv.html"
export PYTHONPATH=SPYTHONPATH:$SU2_RUN
export MYSTRAN="/home/bcrow/Documents/MYSTRAN_Linux_64"
export PYTHONPATH=SPYTHONPATH:$MYSTRAN
fexport PYTHONPATH=SPYTHONPATH:$MYSTRAN
```

Figure 1: ESPenv.sh file

- 6. After that, you will need to tell the computer where the MYSTRAN Files are located. To do this add these lines to the bottom as well (you should still be in the ESPenv.sh file).
- 7. Here, "path/to/MYSTRAN" is a place-holder for the path to the MYSTRAN_Linux_64 directory.:

export MYSTRAN="path/to/MYSTRAN" export PATH=\$PATH:\$MYSTRAN

- 8. Save your ESPenv.sh file and close out of the editor.
- 9. From the website that you downloaded MYSTRAN, take the "UNLOCK XXXXXXXXXXXXXXX" line and put it in the MYSTRAN.INI file.
 - 1. cd MYSTRAN/MYSTRAN Linux 64
 - 2. Open up MYSTRAN.INI with an editor
 - 3. Add the "UNLOCK XXXXXXXXXXXXXXXXX" line. Make sure that the work UNLOCK starts at column 1 and the 33 digits start at column 9. See Figure 2.
 - 4. Close and save the MYSTRAN.INI file

GNU nano 2.9.3

UNLOCK 243064687785410053590938998052562

Figure 2: MYSTRAN.INI file

10. Finally, add the following lines to the end of your .bashrc file (This step is detailed in the MYSTRAN-Install-Manual under the section "Changing directories where MYSTRAN executable resides" (See figure 3)):

source path_to_MYSTRAN/set_MYSTRAN_directory.sh MYSTRAN_directory=path_to_MYSTRAN

Figure 3: .bashrc file