MicroSim Installation: GUI/ Infile generator/ post-processing tool

Infile generator and post-processing tool

Python GUI application for generating Infile and Filling files, and post-processing tool.

- You can use a package manager like Miniconda or Anaconda to avoid issues with system python. Miniconda is enough for this specific purpose.
- Download and install Miniconda package:

```
cd ~/
wget https://repo.anaconda.com/miniconda/Miniconda3-py310_23.1.0-1-Linux-x86_64.sh
# Install using the following command
bash Miniconda3-py310_23.1.0-1-Linux-x86_64.sh
```

- Now create a virtual environment with python 3.9 (version previous to this are also compatible with the packages required) and pip:

```
conda create --name msenv python=3.9 pip
```

- Activate virtual environment msenv:

```
conda activate msenv
```

- Install the packages below using pip:

```
pip install pyqt5 scikit-image vtk tinydb sympy==1.8 pycalphad==0.9.2 pymks yt
```

  Caution: Run the above pip install command as it is. Installing the packages one at a time will throw up dependency error.

- Launch MicroSim GUI:

```
python3 MicroSim.py
```

To use h5 to vtk converter in post-processing:

Download and extract ParaView:

```
cd $HOME
wget "https://www.paraview.org/paraview-downloads/download.php?submit=Download&version
=v5.10&type=binary&os=Linux&downloadFile=ParaView-5.10.1-MPI-Linux-Python3.9-x86_64.ta
r.gz"
tar -zxvf ParaView-5.10.1-MPI-Linux-Python3.9-x86_64.tar.gz
echo 'export PATH="$HOME/ParaView-5.10.1-MPI-Linux-Python3.9-x86_64/bin:$PATH"' >> ~/.
bashrc
```

Install openmpi version > 4.0.0:

1. Ubuntu-20.04 or higher:

   ```
   sudo apt-get update
   sudo apt install build-essential
   sudo apt-get install gcc
   sudo apt-get -y install openmpi-bin openmpi-doc libopenmpi-dev
   ```

2. Ubuntu-18.04:

   Install from source:

   ```
   sudo apt-get install gcc
   sudo apt-get install openmpi-bin openmpi-common libopenmpi-dev
   cd ~/
   sudo wget https://www.open-mpi.org/software/ompi/v4.1/downloads/openmpi-4.1.1.tar.
   gz
   sudo tar -xvzf ~/openmpi-4.1.1.tar.gz
   cd openmpi-4.1.1
   sudo ./configure --prefix="/opt/openmpi-4.1.1"
   sudo make
   sudo make install

   echo 'export PATH=”$PATH:/opt/openmpi-4.1.1/bin”' >> ~/.bashrc
   echo 'export LD_LIBRARY_PATH=”$LD_LIBRARY_PATH:/opt/openmpi-4.1.1/lib”' >> ~/.bash
   rc

   source ~/.bashrc
   ```

   ```
   # find the location of libmpi.so:
   whereis libmpi.so
   ```

```
# on my system output is: libmpi: /usr/lib/x86_64-linux-gnu/libmpi.so
# create a symbolic link for libmpi.so.40 at this location
sudo ln -s /opt/openmpi-4.1.1/libmpi.so.40 /usr/lib/x86_64-linux-gnu/
```

Note: Every time you open a new terminal and want to launch MicroSim Infile generator/GUI, you need to run the following command:

```
conda activate msenv
```