MicroSim Installation: Singularity and Grand-Potential solver

1. Install singularity from GitHub according to your OS-version:-

   a. Ubuntu 18.04:

   ```
   cd ~/
   wget https://github.com/sylabs/singularity/releases/download/v3.11.3/singularity-ce_3.11.3-bionic_amd64.deb
   sudo apt install -y ./singularity-ce_3.11.3-bionic_amd64.deb
   ```

   b. Ubuntu 20.04:

   ```
   cd ~/
   wget https://github.com/sylabs/singularity/releases/download/v3.11.4/singularity-ce_3.11.4-focal_amd64.deb
   sudo apt install -y ./singularity-ce_3.11.4-focal_amd64.deb
   ```

   c. Ubuntu 22.04:

   ```
   cd ~/
   wget https://github.com/sylabs/singularity/releases/download/v3.11.4/singularity-ce_3.11.4-jammy_amd64.deb
   sudo apt install -y ./singularity-ce_3.11.4-jammy_amd64.deb
   ```

2. Download the MicroSim package from GitHub repository:

   https://github.com/ICME-India/MicroSim/archive/refs/heads/main.zip

   ```
   cd ~/
   wget https://github.com/ICME-India/MicroSim/archive/refs/heads/main.zip
   unzip main.zip
   ```

3. If you have a pre-built singularity image then skip to step 4.

   If you do not have a pre-built image, then to build singularity image by running the following command in the terminal:

   ```
   # Go to the folder where def file is located, then run the following command
   sudo singularity build GP_GUI.sif MicroSim-main/def_files/GP_GUI.def
   # This will generate a GP_GUI.sif file. Move this file to a folder which contains MicroSim
   ```

4. Run the following command in terminal (so that Grand-Potential solver can be used via GUI)

   ```
   cd MicroSim-main
   sh swap_script.sh
   cd ..
   ```

5. To load the image in singularity and open singularity terminal:

```
# Following command has to be run from the folder which contains GP_GUI.sif and MicroSim both
singularity shell --bind /run/user,./MicroSim-main:/mnt GP_GUI.sif
```

6. Go to the MicroSim folder using the following command:

```
cd /mnt
```

7. Running MicroSim from terminal:

```
# Go to the Grand potential solver directory
cd Grand_potential_Finite_difference_2D_MPI

#clean the old compiled files
make clean

#compile the solver
make

# Run the solver on 4 cores
mpirun -np 4 ./microsim_gp Input_tdb_new.in Filling.in outputname 2 2
```