

MicroSim Installation procedure for Singularity and Grand-Potential solver

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

- a. Ubuntu 18.04:

https://github.com/sylabs/singularity/releases/download/v3.11.3/singularity-ce_3.11.3-bionic_amd64.deb

- b. Ubuntu 20.04:

https://github.com/sylabs/singularity/releases/download/v3.11.4/singularity-ce_3.11.4-focal_amd64.deb

- c. Ubuntu 22.04:

https://github.com/sylabs/singularity/releases/download/v3.11.4/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>

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: (**Sudo permission are needed for building**)

```
# Go to the folder where def file is located, then run the following command
sudo singularity build GP_GUI.sif 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)

```
# Go to MicroSim folder and run:
sh ./swap_script.sh
```

To revert back the settings:

```
sh ./swapback_script.sh
```

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 ./MicroSim:/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
```

8. To open the GUI:

```
# Go to the MicroSim folder and run the following command:
python3 MicroSim.py
```