The MATLAB workflow is as follows:

1. Generate the electrodes and their mesh with “Main_Stochastic_Generation.m”
2. Extract observables with “Main_Extracting_Electrodes_Observables.m”
3. Once all the COMSOL simulations are done, use “Main_COMSOL_PostProcessing.m” to automatically extract the observables from the .mph files

To use the MATLAB scripts, you just need to fill the necessary parameters (highlighted by “INPUTS” sections) and then to run the codes. To mesh, you will need to have installed Iso2mesh (https://iso2mesh.sourceforge.net/cgi-bin/index.cgi), as well as TauFactor (https://www.mathworks.com/matlabcentral/fileexchange/57956-taufactor) for the extraction of observables. For the latter, you will need to replace the original “TauFactor.m” file by the modified “TauFactor.m” from this study located in the “Observables Extraction” folder. For Iso2Mesh, need to replace the original “v2m.m” and “vol2mesh.m” files by the one in the folder “Stochastic Generation”.

The workflow of the python script is as follows:

1. Define the function k_fold()
2. Convert the .mat combined SOD+observables files into .pkl
3. Import the desired .pkl files to create the dataset
4. Screening through the number of trees, maximal number of branches per tree, randomization seeds for the training of the Random Forest algorithm, applying the 10-fold approach
5. Training of the optimized Random Forest algorithm based on 4)
6. Visualization of the SHAP values