Application example: Surface plasmon polariton waves on a graphene layer

SIM5G: FDTD toolbox

Surface plasmon polaritons (SPPs) are electromagnetic waves strongly confined at the interface between a conductor and a dielectric, coupled with collective oscillations of surface charges. These waves exhibit unique characteristics, such as strong field confinement and subwavelength propagation, making them highly desirable for applications in sensing, photonics, and integrated optics. Graphene, with its unique electronic properties and tunable conductivity, has emerged as an exceptional platform for supporting SPPs at terahertz to mid-infrared frequencies. In this example, the FDTD method is employed to simulate the propagation of SPP waves on a graphene surface. The simulation highlights key characteristics such as field confinement, propagation length, and dispersion properties, demonstrating the method's efficacy in modeling plasmonic systems.

An overview of the application example is the following

- **Model**: A planar material with infinite dimensions on the $xy-$plane at free-space.
- **Computational Domain**: A cubic FDTD simulation domain of side dimension $200\,\mu$m with absorbing boundary conditions (Perfectly Matched Layers, PML) to simulate an open environment. The cell-to-wavelength ratio is selected 80 to evaluate the sub-wavelength surface waves.
- **Excitation**: A point dipole at graphene's center with direction towards the $z-$axis.
- **Operating Frequency**: A broadband analysis is conducted from 1 to 3 THz.
- **Objective**: Computation and visualization of the electric field to verify the propagation of surface waves.

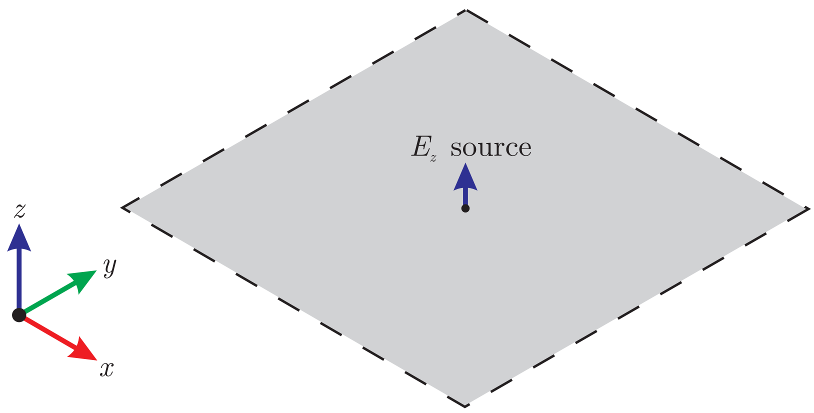


Figure 1: A point source excitation on a planar graphene layer.

1 Setup of the FDTD simulation

To address the described scenario effectively, the SIM5G FDTD toolbox provides a versatile framework for simulating electromagnetic phenomena. All electromagnetic interactions can be simulated with precision by systematically applying its modules, as depicted in Fig. 2. The following sections outline the specific steps used in each analysis stage.

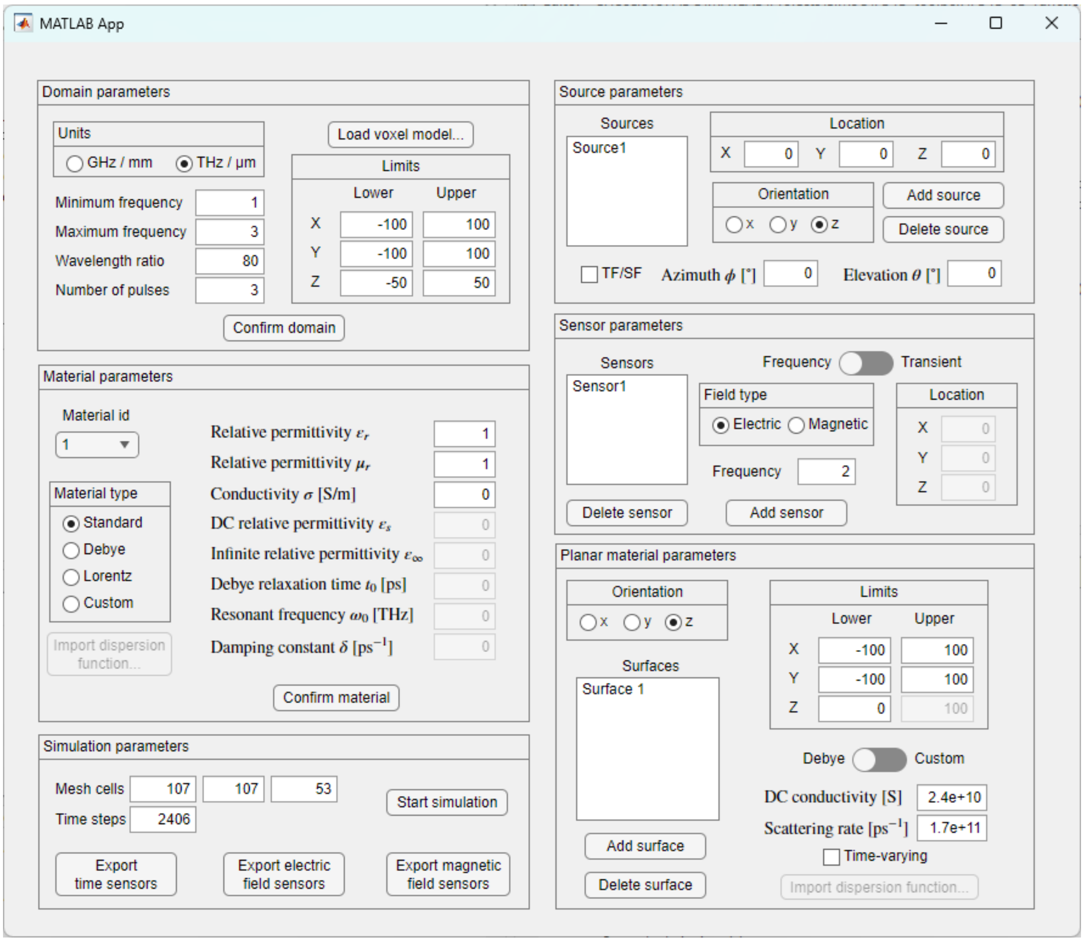


Figure 2: Overview of the SIM5G FDTD toolbox for the simulation of the scatterer.

1.1 Domain parameters

- **Load voxel model**: A file dialog opens, and ".\Models\voxel_model_free-space.mat" shall be selected to load the model to be simulated.
- **Units**: The option "THz/mm" shall be selected.
- **Minimum frequency**: It shall be set to 1 THz (the unit is automatically applied).
- **Maximum frequency**: It shall be set to 3 THz (the unit is automatically applied).
- **Number of pulses**: Normally, more than 3 shall be selected. However, 3 is adequate for this problem.

- **Limits**: The lower limit shall be set $-100\,\mu$m and the maximum $100\,\mu$m for x and y directions. Along $z-$axis the values shall be set $-50\,\mu$m and $50\,\mu$m, correspondingly (all the units are automatically applied).
- **Confirm domain**: After setting all the parameters, the domain shall be confirmed with this button. This will enable the material selection for the model and initiate the simulation parameters.

1.2 Material parameters

For material with id$=1$:

- This material is air, which has the default parameters. For this reason, no further action is required.

1.3 Source parameters

- **Location**: The center of the computational domain, namely at the position $x = 0\,\mu$m, $y = 0\,\mu$m and $z = 0\,\mu$m (the unit is automatically applied).
- **Orientation**: The option "z" shall be selected.
- **Add source**: After setting the excitation parameters, the source shall be confirmed with this button.

1.4 Sensor parameters

- **Frequency**: The toggle button shall be set to this option.
- **Field type**: The option "Electric" shall be selected.
- **Frequency**: It shall be set to 2 THz (the unit is automatically applied).
- **Add sensor**: After setting the electric sensor parameters, it shall be confirmed with this button.

1.5 Planar material parameters

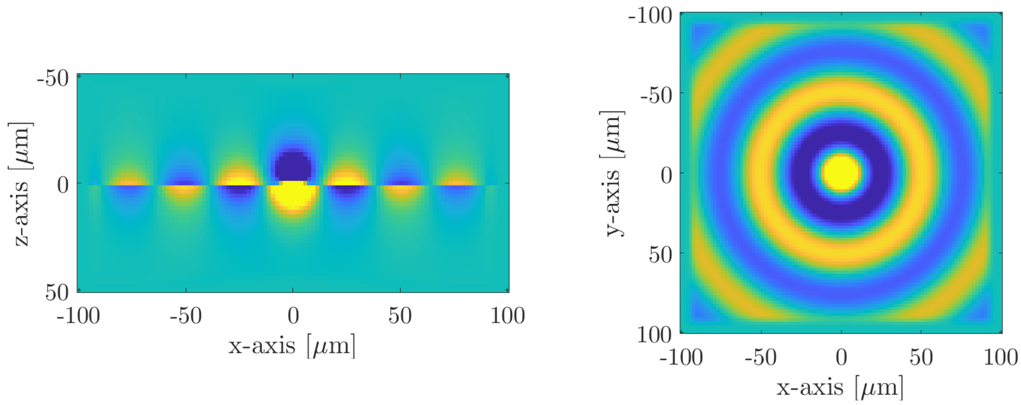
- **Orientation**: The option z shall be selected, which indicates the normal vector of the surface.
- **Limits**: The planar surface lies on the entire computational domain. As a result, the lower limit shall be set $-100\,\mu$m and the maximum $100\,\mu$m for x and y directions at $z = 0\,\mu$m (all the units are automatically applied).
- **Debye**: The toggle button shall be set to this option.
- **DC conductivity**: The value $2.4 \cdot 10^{10}$ S shall be selected corresponding to a chemical potential 0.2 eV.
- **Scattering rate**: The value $1.7 \cdot 10^{11}$ ps^{-1} shall be selected corresponding to 0.11 meV.

1.6 Simulation parameter

- The "Mesh cells" and the "Time steps" shall be automatically retrieved by confirming the previous steps.
- **Start simulation**: The FDTD simulation will start with this button.
- After the simulation is completed, the results can be exported with the button "Export electric field sensors".

2 Results of the FDTD simulation

The results are saved inside the application's folder with the name "FDTDxxfieldSensor.txt", where "xx" corresponds to the field component, namely "FDTDexfieldSensor.txt" corresponds to E_x. The results are saved into a vector form using two columns per monitor, one for the real and one for the imaginary part. Initially, the complex form shall be retrieved, while to acquire the voxel-based values one shall use the command:
`B = reshape(A, N, M, K)`
where `A` is the complex values in vector form, `B` the desired complex values in the voxel-based form and `N, M, K` are mesh cells along each direction, which can be derived by the FDTD toolbox under the "Simulation parameters" tab. Finally, the distribution of the E_z component at the xz and $xy-$planes is visualized in Fig. 3, indicating the strong confinement on the graphene surface and the sub-wavelength nature of the surface waves (free-space wavelength $\lambda_0 = 150\,\mu$m and surface plasmon polariton wavelength $\lambda_{\text{SPP}} \approx 50\,\mu$m at 2 THz).



(a) $xz-$plane ($y = 0$) (b) $xy-$plane ($z = 0$)

Figure 3: Distribution of the E_z component at different planes for the surface wave propagation on graphene at 2 THz.