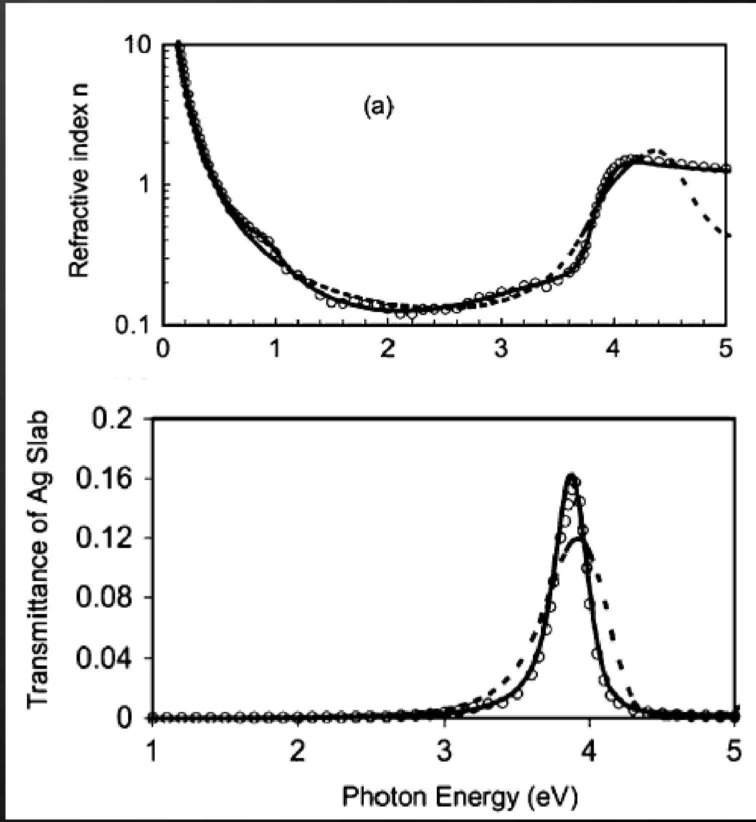
FDTD IN DISPERSIVE MEDIA: COMPLEX-CONJUGATE POLE-RESIDUE PAIRS METHOD

Dispersive material: waves of different frequencies travel at different velocities

- **How do we model the media?**



María Pedrosa Bustos

Computational Methods in Non-Linear Physics - FisyMat

MODEL

permittivity as the sum of complex-conjugate pole-residue pairs

$$\varepsilon(\omega) = \varepsilon_0\varepsilon_\infty + \varepsilon_0 \sum_{p=1}^{P} c_p/(j\omega - a_p) + c_p^*/(j\omega - a_p^*)$$

Real part of a_p **must** be **negative**

$$\vec{J}_p(\omega) = \varepsilon_0 \frac{c_p}{j\omega - a_p} j\omega \vec{E}(\omega)$$
$$\vec{J}_p'(\omega) = \varepsilon_0 \frac{c_p^*}{j\omega - a_p^*} j\omega \vec{E}(\omega).$$

$$\frac{d}{dt}\vec{J}_p(t) - a_p \vec{J}_p(t) = \varepsilon_0 c_p \frac{d}{dt}\vec{E}(t)$$
$$\frac{d}{dt}\vec{J}_p'(t) - a_p^* \vec{J}_p'(t) = \varepsilon_0 c_p^* \frac{d}{dt}\vec{E}(t).$$

Maxwell equations

$$\vec{\mathcal{D}} = \varepsilon\vec{\mathcal{E}}$$
$$\vec{\mathcal{B}} = \mu\vec{\mathcal{H}}$$
$$\vec{\mathcal{J}} = \sigma\vec{\mathcal{E}}$$

Auxiliary differential equation (ADE)

$$\vec{J}_p^{\,n+1/2} = k_p \vec{J}_p^{\,n-1/2} + \beta_p \left(\frac{\vec{E}^{\,n+1/2} - \vec{E}^{\,n-1/2}}{\Delta t} \right)$$

$$\vec{E}_{i,j,k}^{n+1/2} = \frac{\varepsilon_{i,j,k} - \sigma_{i,j,k}\Delta t/2}{\varepsilon_{i,j,k} + \sigma_{i,j,k}\Delta t/2} \vec{E}_{i,j,k}^{n-1/2} + \frac{\Delta t}{\varepsilon_{i,j,k} + \sigma_{i,j,k}\Delta t/2} \tilde{\delta}_r \vec{H}_{i,j,k}^{n}$$
$$\vec{H}_{i,j,k}^{n+1} = \vec{H}_{i,j,k}^{n} - \frac{\Delta t}{\mu_{i,j,k}} \tilde{\delta}_r \vec{E}_{i,j,k}^{n+1/2}$$

$$\vec{E}^{\,n+1/2} = \left(\frac{2\varepsilon_0\varepsilon_\infty + \sum_{p=1}^{P} 2\mathrm{Re}(\beta_p) - \sigma\Delta t}{2\varepsilon_0\varepsilon_\infty + \sum_{p=1}^{P} 2\mathrm{Re}(\beta_p) + \sigma\Delta t} \right) \vec{E}^{\,n-1/2} + \frac{2\Delta t \cdot \left[\nabla \times \vec{H}^{\,n+1} - \mathrm{Re}\sum_{p=1}^{P} (1+k_p)\vec{J}_p^{\,n-1} \right]}{2\varepsilon_0\varepsilon_\infty + \sum_{p=1}^{P} 2\mathrm{Re}(\beta_p) + \sigma\Delta t}$$

$$k_p = \frac{1 + a_p\Delta t/2}{1 - a_p\Delta t/2}$$

$$\beta_p = \frac{\varepsilon_0 c_p \Delta t}{1 - a_p\Delta t/2}$$

$$\vec{H}^{n+1} = \vec{H}^{n} - \frac{\Delta t}{\mu} \tilde{\delta}_r \vec{E}^{n+1/2}$$

Same as Yee algorithm

saves memory space and CPU time consumption

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- **How do we model the media?**
- **How do we measure the results?**

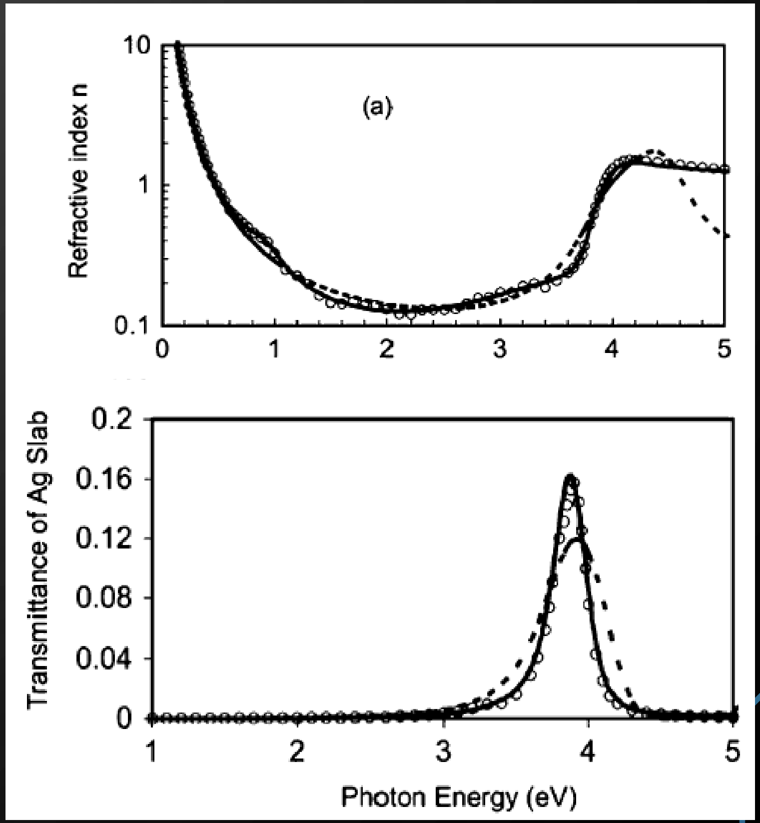
Transmission/reflection coefficient -> ratio of the transmitted/reflected to incident electric field

$$\mathrm{T} = \frac{|E_t(\omega)|}{|E_i(\omega)|}$$

Transmittance -> fraction of the power that transmits

$$reflectance = \frac{P_t(\omega)}{P_i(\omega)} = \frac{|E_r(\omega)|^2}{|E_i(\omega)|^2}$$

$$transmittance = 1 - reflectance$$



CODE

New Class for layer properties

dispersiveMedia.py

- Stores ε_∞, μ, a_p, c_p, layer width and position
- Changes units of frequency
- Calculate layer's coordenates
- Calculate c_p, k_p

Changes in viewer

- Display layer
- Show both dispersed and free space solution

Problems:

- Need to save solution for dispersive and non dispersive media.
- Be careful with the units range!

Changes in solver

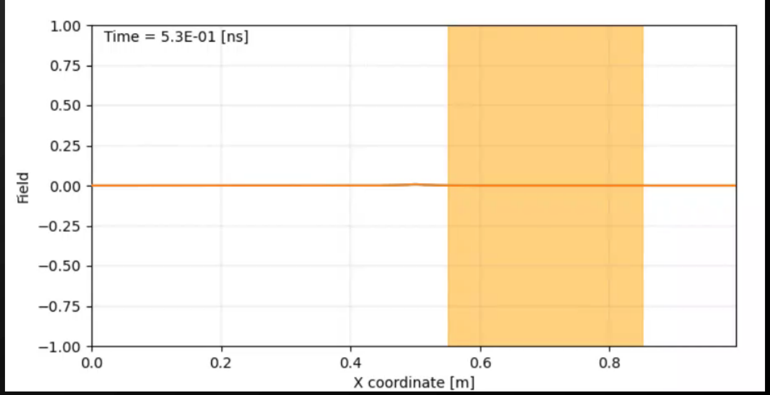
- Add ADE equations to updateE. Two methods:
  - Array of permittivities
  - Only apply at certain índices
- Also added μ option
- Saves both dispersed and free space solutions

Measurements: new class

Transmittance.py

- Computes numerical T and R, transmittance and reflectance (using FFT)
- Computes analytical T and R
- Plot the results.

$$\varepsilon_\infty = 5$$
$$d = 0.1\ m$$
$$t_{max} = 5.6\ ns$$
$$G_{spread} = 0.25\ ns$$



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- D.W. Lynch andW. R. Hunter. (1985). *Handbook of Optical Constants of Solids*, E. D. Palick, Ed. Orlando, FL: Academic,

THE END

tests\cavity_dispersive_test.json

```
"finalTime": 20e-9,
"cfl": 1
"coordinates": [
    0.0,
    1.5,
"grid": {
    "elemId": 0,
    "steps": 0.001,
    "bounds": ["mur", "mur"]
},
"sources": [
    {
        "type": "dipole",
        "direction": [0.0, 0.0,
        "magnitude": {
            "type": "gaussian",
            "gaussianDelay": 1.
            "gaussianSpread": 0.
        },
        "elemId": 1
    }
],
"dispersiveLayers":
    {
        "permittivity": 1.2,
        "permeability":1,
        "ap": [
            "-2.502e-2-8.626e-3j",
            "-2.021e-1-9.407e-1j",
            "-1.467e1-1.338j",
            "-2.997e-1-4.034j",
            "-1.896-4.808j",
            "-9.396-6.477j"
        ],
        "cp": [
            "5.987e-1+4.195e3j",
            "-2.211e-1+2.680e-1j",
            "-4.240e...",
            "6.391e-1-7.186e-2j",
            "1.806+4.563j",
            "1.443-8.219e1j"
        ],
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        "width": 1
    },
```
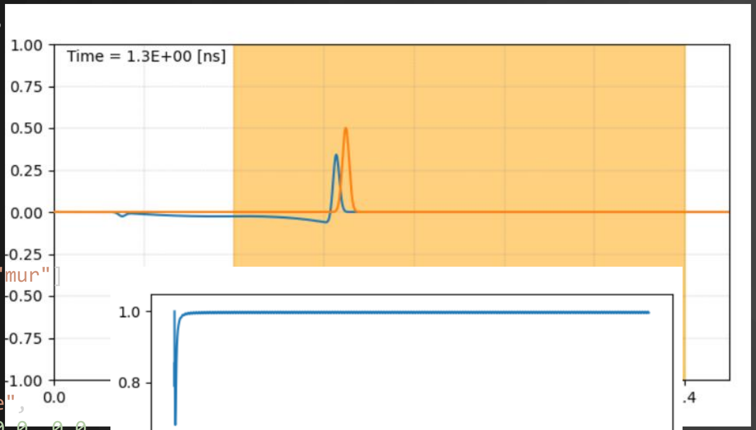
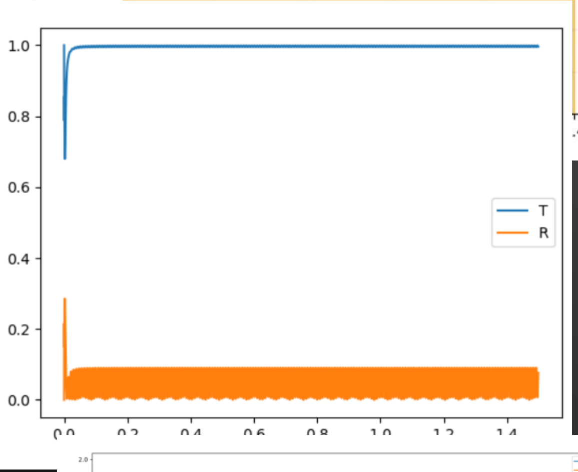
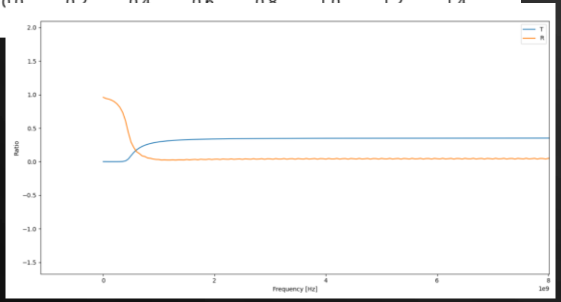
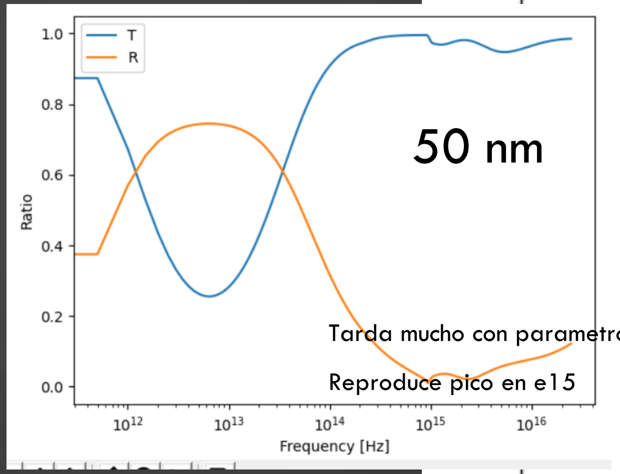







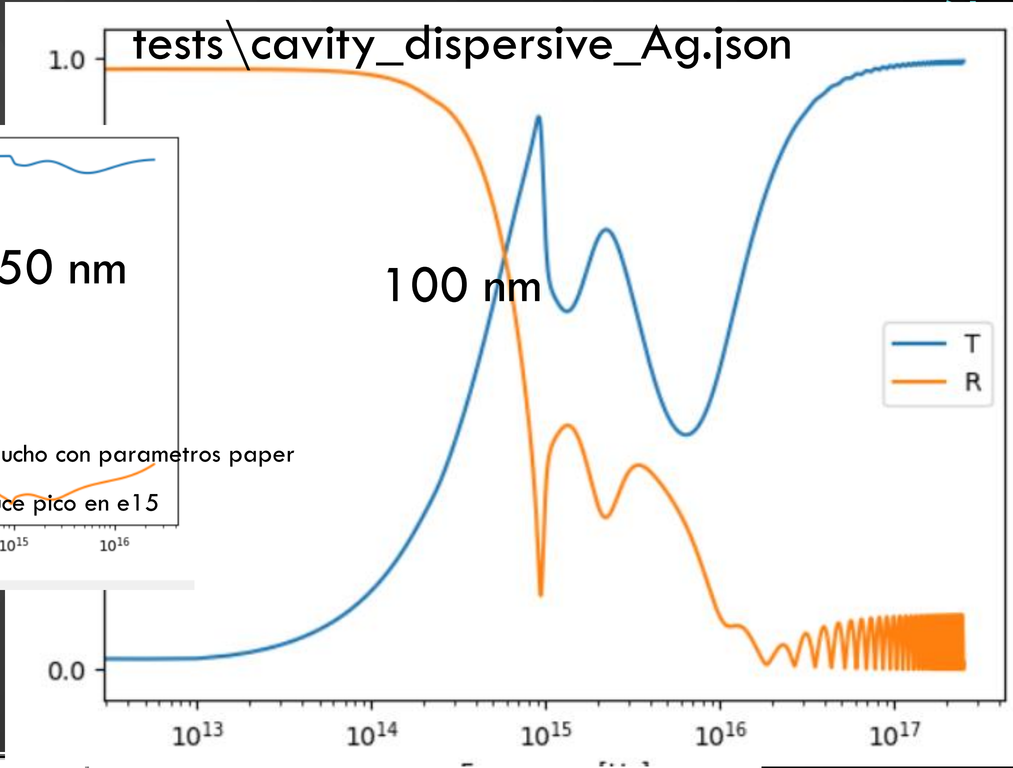
tests\cavity_dispersive_Ag.json



50 nm

Tarda mucho con parametros paper

Reproduce pico en e15



100 nm

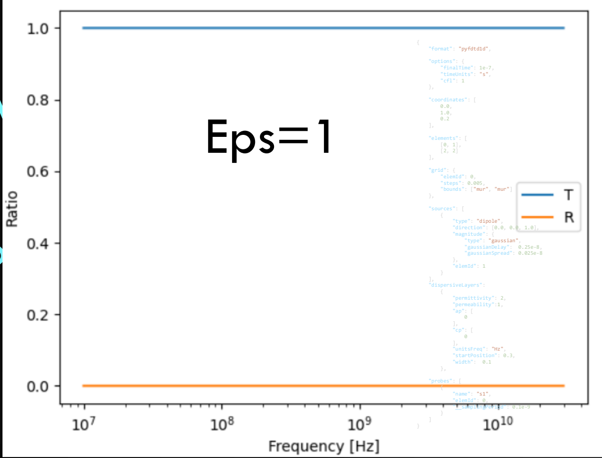
Parameters	*Values (unit:eV)*
(c_1, a_1)	$(5.987\times10^{-1}+j4.195\times10^{3},\ -2.502\times10^{-2}-j8.626\times10^{-3})$
(c_2, a_2)	$(-2.211\times10^{-1}+j2.680\times10^{-1},\ -2.021\times10^{-1}-j9.407\times10^{-1})$
(c_3, a_3)	$(-4.240+j7.324\times10^{2},\ -1.467\times10^{1}-j1.338)$
(c_4, a_4)	$(6.391\times10^{-1}-j7.186\times10^{-2},\ -2.997\times10^{-1}-j4.034)$
(c_5, a_5)	$(1.806+j4.563,\ -1.896-j4.808)$
(c_6, a_6)	$(1.443-j8.219\times10^{1},\ -9.396-j6.477)$

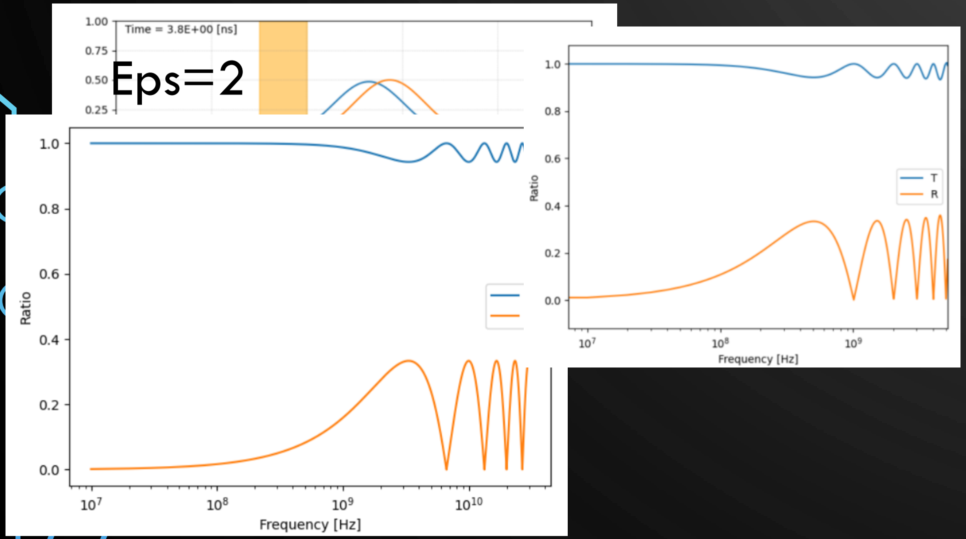
High frequencies where wavelength similar to grid spacing => error in Fouriier

Can not set values <1 in eps infitity

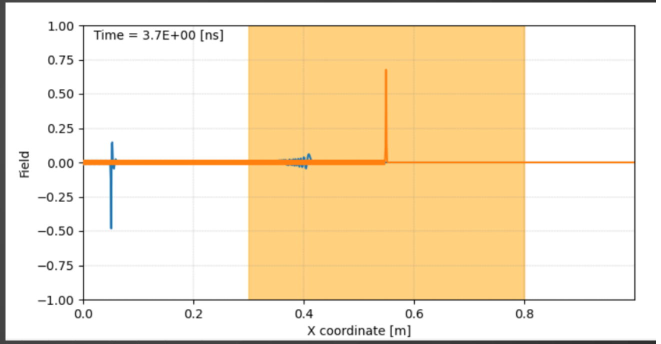
Can not start source very soon

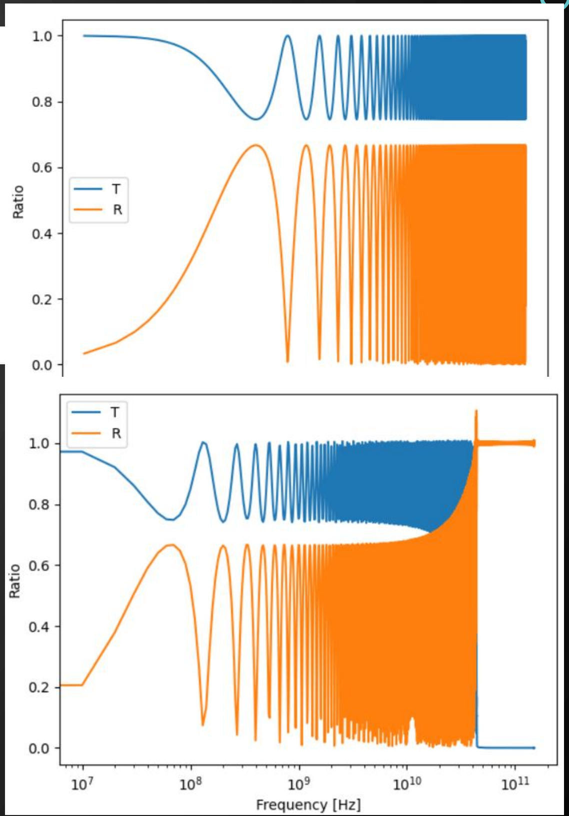
tests\cavity_dispersive_test_NoComplex.json





tests\cavity_dispersive_test_NoComplex_ShortDipole.json



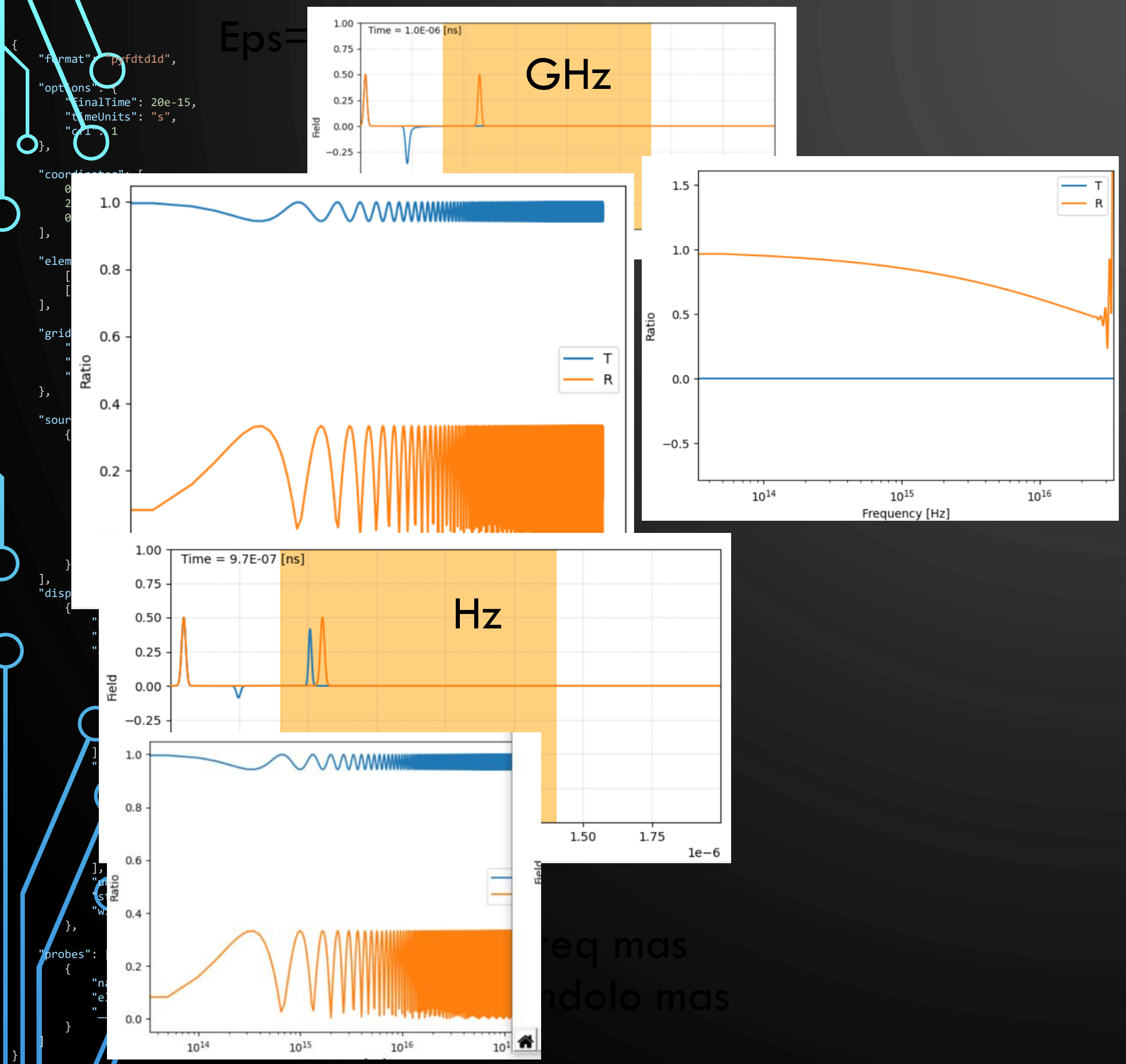


Revota hacia atrás

Los picos no a la misma freq => creo que es por el Fourier, porque quita como una década (por donde aparece el ruido en Fourier

Delay pequeño va mal

tests\cavity_dispersive_test_ShortDipole .json

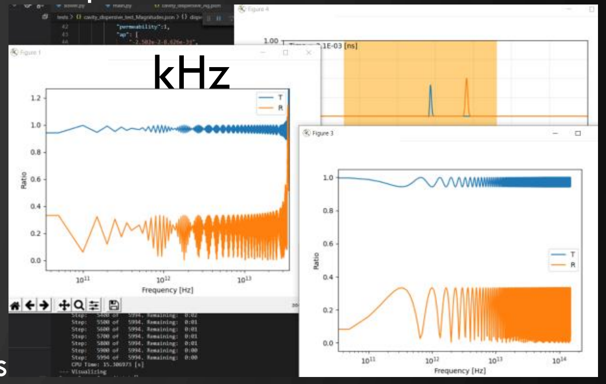


tests\cavity_dispersive_test_Magnitude.json

"steps": 0.001e-3 y Ghz, => paso temporal demasiado grande

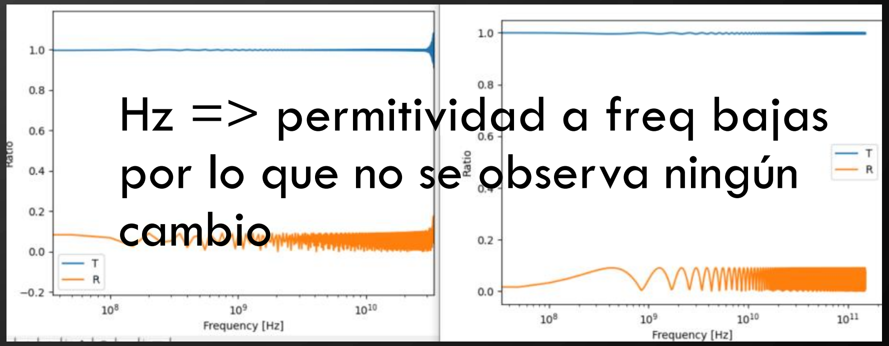
Jugar con:

- Tamaño grid
- Freq.
- Spacing
- Tiempo renderizado

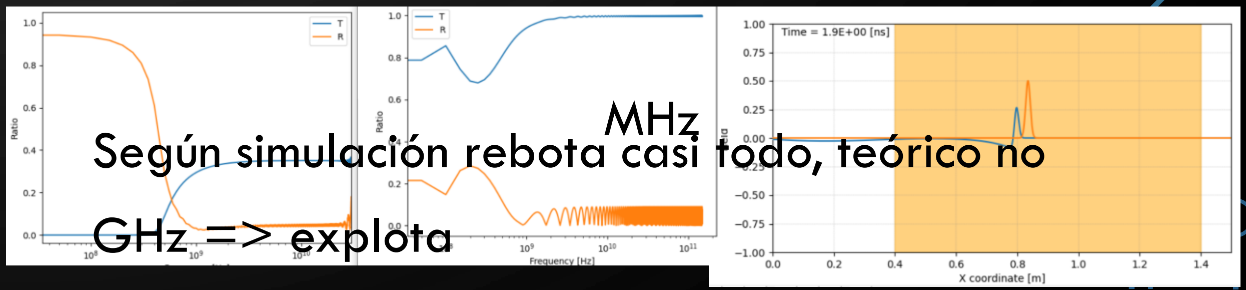


Freq pequeñas => tiempos largos
spacing grande =>ajustar Tambien eps

tests\cavity_dispersive_test_Both.json



Hz => permitividad a freq bajas por lo que no se observa ningún cambio



Según simulación rebota casi todo, teórico no

GHz => explota

CLASE APARTE?

VARIAS WALLS

NO PUEDE SER DE 1NM, ES MUY PEQUEÑO!!

NORMALIZAR FREC.

FUNCION COMPLEXFIELD EN DISPERSIVE MEDIA??

COPY.DEEPCOPY PARA NO CARGARTE LA CLASE?

POR Q LA FUNCION FIELDS?

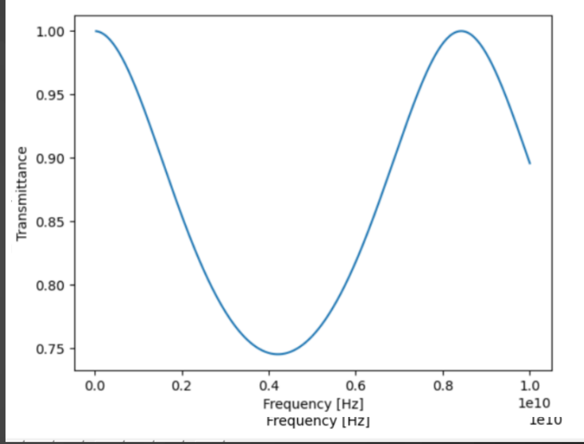
LINEA SOLVER DEBAJO FOR I IN RANGE(0,NP.SHAPE(JP_OLD)[1]): . NO PONGO 1:-1? AL JP?

INDICES DE H Y E CON CUAL CORRESPONDEN?

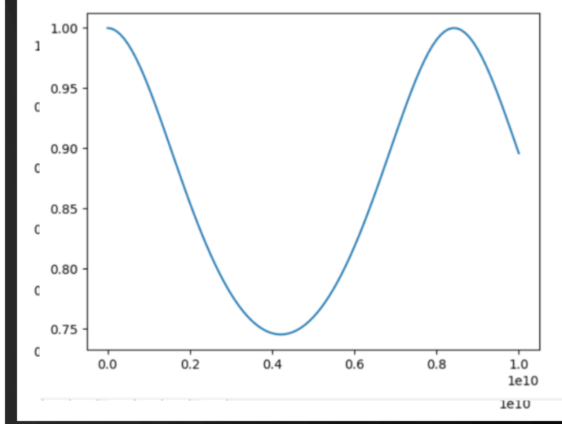
FFT.FFTSHIFT?

DIFERENCIA EPS_INF Y EPS_R

CALCULAR DISPERSIVE Y NO EN SOLVER? O QU CALCULE

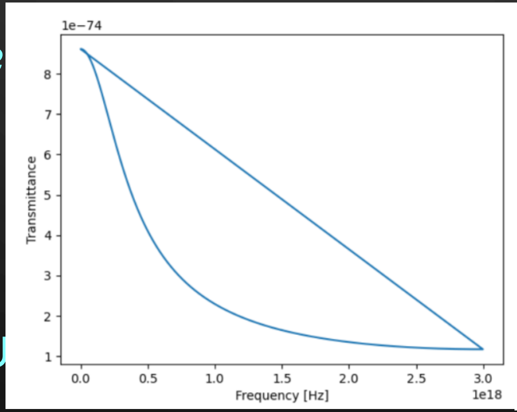


My class =>eps=5, ap=cp=0,width =>



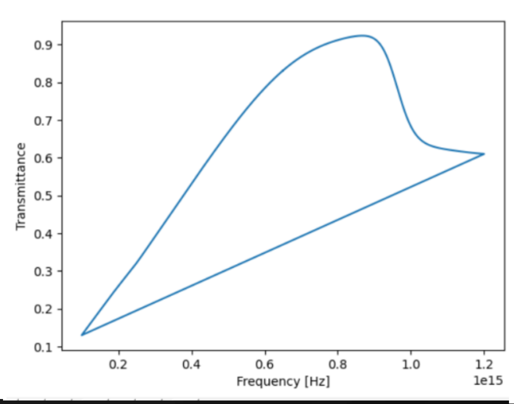
angulo=>eps=5, ap=cp=0

Numerical Ag 1nm



My class analytic Ag

100 nm



My class analytic Ag

1 nm