

Hello All,

I'm investigating the scatter properties of nano antennas by using the scattering formulation in the RF module. I start from two nano spheres, and attached please find the .mph files. In the model, Domains 19 and 20 are nano spheres, which have complex permittivities given by Drude model. The nano particles are put in Domain 14, which is an air box and is bounded by PMLs. I know I can use the predefined Drude material type to represent the nano-spheres and it works great without doubts. However, I need to modify the weak form in someway later, so I go to the equation view and find that the predefined weak form for the equation

$$\nabla \times \mu_r^{-1}(\nabla \times \mathbf{E}) - k_0^2(\epsilon_r - \frac{j\sigma}{\omega\epsilon_0})\mathbf{E} = 0 \quad (1)$$

is

$$-\mu_0\_const * (-emw.dHdtx*emw.curltestdepEx - emw.dHdty*emw.curltestdepEy - emw.dHdtz*emw.curltestdepEz + emw.iomega * (emw.Jx*emw.testdepEx + emw.Jy*emw.testdepEy + emw.Jz*emw.testdepEz))$$

However, when I write the weak form of Eq. (1) directly, I think it reads

$$\int_{\Omega} \left[ \mu_r^{-1}(\nabla \times \mathbf{E}) \cdot (\nabla \times \mathbf{V}) - k_0^2(\epsilon_r - \frac{j\sigma}{\omega\epsilon_0})\mathbf{E} \cdot \mathbf{V} \right] d\Omega = 0 \quad (2)$$

where  $\mathbf{V}$  is the test function, and I chose it to be  $\mathbf{E}^{sca}$ . So, I rewrite the weak form into COMSOL like this

$$(emw.curlEx*test(curlEx) + emw.curlEy*test(curlEy) + emw.curlEz*test(curlEz)) / mur - (emw.k0)^2 * (epsr + sigma0/emw.iomega/epsilon0_const) * (emw.Ex*test(emw.relEx) + emw.Ey*test(emw.relEy) + emw.Ez*test(emw.relEz))$$

and it gives me nothing (the calculated result is a uniform normE-field distribution in the whole domain except PMLs). However, if I negative the above weak form, say

$$-((emw.curlEx*test(curlEx) + emw.curlEy*test(curlEy) + emw.curlEz*test(curlEz)) / mur - (emw.k0)^2 * (epsr + sigma0/emw.iomega/epsilon0_const) * (emw.Ex*test(emw.relEx) + emw.Ey*test(emw.relEy) + emw.Ez*test(emw.relEz)))$$

I get the correct solution. Why? It does not make sense to me. So, my question is: **how can I get the correct weak form of a PDE for COMSOL?**

Now, let's move to the next question regarding the coupling physics in COMSOL. I want to couple the following two PDEs for nanospheres[1, 2], say, in the domains 19 and 20,

$$\nabla \times \nabla \times \mathbf{E} - \epsilon_{inf} k_0^2 \mathbf{E} = -j\omega\mu_0 \mathbf{J} \quad (3a)$$

$$\beta^2 \nabla(\nabla \cdot \mathbf{J}) + (\omega^2 - j\omega\gamma) \mathbf{J} = -j\omega\epsilon_0 \omega_p^2 \mathbf{E} \quad (3b)$$

where the boundary condition for the phasor current  $\mathbf{J}$  is  $\mathbf{n} \cdot \mathbf{J} = 0$ , at the boundaries of the nanoparticles. So I added a *Weak Form PDE* physic environment for the phasor current to the *Electromagnetic Wave, Frequency Domain*

environment for  $\mathbf{E}$ ; and named the *Field Name* of the *Weak Form PDE* model to be  $Jh$ , which has three dependent variables  $Jh1$ ,  $Jh2$  and  $Jh3$ , respectively. Then, I input the weak form for the scatter field in the *Electromagnetic Wave, Frequency Domain* physics, as

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-(emw.curlEx*test(curlEx)+emw.curlEy*test(curlEy)+emw.curlEz*test(
curlEz))+epsinf*(emw.k0)^2*(emw.Ex*test(emw.relEx)+emw.Ey*test(
emw.relEy)+emw.Ez*test(emw.relEz))-emw.iomega*mu0_const*(Jh1*
test(emw.relEx)+Jh2*test(emw.relEy)+Jh3*test(emw.relEz))
```

and for the phasor current  $Jh$  in the *Weak Form PDE* physics, as

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beta^2*(Jh1x+Jh2y+Jh3z)*test(Jh1x)-(omega0^2-1i*omega0*gamma)*Jh1*
test(Jh1)-1i*omega0*epsilon0_const*omegap^2*emw.Ex*test(Jh1)
beta^2*(Jh1x+Jh2y+Jh3z)*test(Jh2y)-(omega0^2-1i*omega0*gamma)*Jh2*
test(Jh2)-1i*omega0*epsilon0_const*omegap^2*emw.Ey*test(Jh2)
beta^2*(Jh1x+Jh2y+Jh3z)*test(Jh3z)-(omega0^2-1i*omega0*gamma)*Jh3*
test(Jh3)-1i*omega0*epsilon0_const*omegap^2*emw.Ez*test(Jh3)
```

and a Constraint at the first component of  $R$

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nx*Jh1+ny*Jh2+nz*Jh3
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as the boundary condition. Unfortunately, it seems to me the two PDEs are not coupled. Could please take a look and see what's the problem?

By the way, I did not experience any problems when using the above techniques for 2D nano wires.

## References

- [1] Giuseppe Toscano, Søren Raza, Antti-Pekka Jauho, N Asger Mortensen, and Martijn Wubs. Modified field enhancement and extinction by plasmonic nanowire dimers due to nonlocal response. *Optics Express*, 20(4):4176–4188, 2012.
- [2] Tianyu Dong, Xikui Ma, and Raj Mittra. Optical response in subnanometer gaps due to nonlocal response and quantum tunneling. *Applied Physics Letters*, 101(23):3111, 2012.