Interpolating between two dispersive media with FDTD adjoint calculations

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As described in the Meep documentation, we can model the permittivity distribution using

$$\epsilon(\omega, \mathbf{x}) = (1 + \frac{i\sigma_D(\mathbf{x})}{\omega})(\epsilon_\infty + \sum_n \frac{\sigma_n(\mathbf{x})\omega_n^2}{\omega_n^2 - \omega^2 - i\omega\gamma_n}). \quad (1)$$

When interpolating between two materials, each may contain their own susceptibilities. We can weight each susceptibility using the interpolation weight u, just like we do with non dispersive media. Specifically, each piece of the above equation now becomes

$$\epsilon_\infty = \epsilon_{\infty_\mathbf{1}} + u(\epsilon_{\infty_\mathbf{1}} - \epsilon_{\infty_\mathbf{0}}) \quad (2)$$

$$\epsilon_{\mathbf{sus}} = (1-u)\sum_n \frac{\sigma_n(\mathbf{x})\omega_n^2}{\omega_n^2 - \omega^2 - i\omega\gamma_n} + (u)\sum_m \frac{\sigma_m(\mathbf{x})\omega_m^2}{\omega_m^2 - \omega^2 - i\omega\gamma_m} \quad (3)$$

where 0 and 1 subscripts correspond to the first and second materials respectively. We also need to create an artificial damping term needed to correct for any accidental zero crossings in the dispersion profile

$$\sigma_D(\mathbf{x}) = u(1-u)\bar{\omega} \quad (4)$$

where $\bar{\omega}$ is the mean resonance frequency of all the susceptibilities.

It's important to note that ϵ_∞, σ_D, and σ are 3×3 *tensors*. We can rewrite our final interpolated permittivity function as a product of two 3×3 matrices, A and B

$$\epsilon(\omega, \mathbf{x}) = A(\omega, \mathbf{x}, u)B(\omega, \mathbf{x}, u) \quad (5)$$

where A is defined as

$$A(\omega, \mathbf{x}, u) = 1 + \frac{u(1-u)\bar{\omega}}{\omega} \quad (6)$$

and B is defined as

$$B = \epsilon_{\infty_\mathbf{1}} + u(\epsilon_{\infty_\mathbf{1}} - \epsilon_{\infty_\mathbf{0}}) + (1-u)\sum_n \frac{\sigma_n(\mathbf{x})\omega_n^2}{\omega_n^2 - \omega^2 - i\omega\gamma_n} + (u)\sum_m \frac{\sigma_m(\mathbf{x})\omega_m^2}{\omega_m^2 - \omega^2 - i\omega\gamma_m} \quad (7)$$

Now, let's remember that the (simplified) gradient leveraging the corresponding adjoint formulation is defined as

$$\frac{df}{d\mathbf{u}} = -\lambda^{\mathbf{H}} C_{\mathbf{u}} \mathbf{x} \tag{8}$$

where f is the objection function, u us once again the vector of design variables, λ is the adjoint field vector, $\mathbf{x}$ is the forward field vector, and $C_{\mathbf{u}}$ is the derivative of the linear operator C w.r.t. the design field.

In our case, the FDFD linear operator (approximated by our hybrid FDTD frequency domain adjoint solver) relates the input and output fields using the permittivity tensor $\epsilon(\omega, \mathbf{x}, \mathbf{u})$. Consequently, the derivative of said tensor w.r.t. $\mathbf{u}$ at one point u is simply

$$C_u = \frac{d\epsilon(\omega, \mathbf{x}, u)}{du} = A\frac{dB}{du} + \frac{dA}{du}B \tag{9}$$

We can calculate each respective derivative for A

$$\frac{dA}{du} = \frac{(1-2u)\bar{\omega}}{\omega} \tag{10}$$

and B

$$\frac{dB}{du} = \epsilon_{\infty_{\mathbf{1}}} - \epsilon_{\infty_{\mathbf{0}}} - \sum_n \frac{\sigma_n(\mathbf{x})\omega_n^2}{\omega_n^2 - \omega^2 - i\omega\gamma_n} + \sum_m \frac{\sigma_m(\mathbf{x})\omega_m^2}{\omega_m^2 - \omega^2 - i\omega\gamma_m}. \tag{11}$$

Each of these calculations will produce a final 3×3 matrix needed to produce a scalar from the two field vectors. Calculating gradients when dealing with dispersive media, therefore, requires a full vector-matrix-vector multiply at each point in space for each frequency of interest. Before, the gradient of the operator C was a constant diagonal matrix, which let us perform a simple, scaled inner product over the adjoint fields and the forward fields.