Driven Solver in Palace

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1 Mathematical Preliminaries

1.1 Governing Equations

Palace solves Maxwell's equations in the frequeny domain (time-harmonic) using a finite element approximation. The non-dimensionalized (complex-valued) equations are

$$\nabla \times \mu_r^{-1} \nabla \times \mathbf{E} + i\omega\sigma\mathbf{E} - \omega^2 \epsilon_r \mathbf{E} = 0,\ \mathbf{x} \in \Omega \tag{1}$$

$$\mathbf{n} \times \mathbf{E} = 0, \mathbf{x} \in \Gamma_{PEC} \tag{2}$$

$$\mathbf{n} \times \mu_r^{-1} \nabla \times \mathbf{E} = 0,\ \mathbf{x} \in \Gamma_{PMC} \tag{3}$$

$$\mathbf{n} \times \mu_r^{-1} \nabla \times \mathbf{E} + \gamma \mathbf{n} \times \mathbf{E} = U^{inc},\ \mathbf{x} \in \Gamma_Z. \tag{4}$$

The relative permittivity ϵ_r is a complex-valued quantity given by $\epsilon_r = \epsilon_r^{'} (1 - i \tan \delta)$. In its current form, Palace only supports a real-valued magnetic permeability $\mu_r = \mu_r^{'}$. The magnetic flux density is calculated as

$$\mathbf{B} = \frac{1}{i\omega} \nabla \times \mathbf{E}. \tag{5}$$

The magnetic flux density and the magnetic field $\mathbf{H}$ are related by the linear constitutive relationship $\mathbf{B} = \mu \mathbf{H}$

The impedance boundaries are modeled using the Robin boundary condition given in Eq. 4 with $\gamma = i\omega / Z_s$ where Z_s is the surface impedance of the boundary. There are other boundary conditions described in but for the moment, this will be the starting point.

1.2 Finite Element Approximation

To arrive at the discrete form of equations, Eq. 1 is multiplied by a test function ν and integrated by parts over the entire domain resulting in the following equation. For clarity, the subscript r is dropped from μ and ϵ.

$$\int_\Omega \nabla \times \left(\mu^{-1} \nabla \times \mathbf{E}\right) \cdot \nu \ d\Omega + \int_\Omega i\omega\sigma\mathbf{E} \cdot \nu \ d\Omega - \int_\Omega \omega^2 \epsilon \mathbf{E} \cdot \nu \ d\Omega = 0 \tag{6}$$

The first term on the LHS can be simplified using the following identity

$$\nabla \cdot \left[(\mu^{-1} \nabla \times \mathbf{E}) \times \nu \right] = \nabla \times (\mu^{-1} \nabla \times \mathbf{E}) \cdot \nu - (\mu^{-1} \nabla \times \mathbf{E}) \cdot (\nabla \times \nu). \quad (7)$$

This results in

$$\begin{aligned} \int_\Omega \nabla \times (\mu^{-1} \nabla \times \mathbf{E}) \cdot \nu \; d\Omega = & \int_\Omega \nabla \cdot \left[(\mu^{-1} \nabla \times \mathbf{E}) \times \nu \right] \; d\Omega \\ & + \int_\Omega (\mu^{-1} \nabla \times \mathbf{E}) \cdot (\nabla \times \nu) \; d\Omega \end{aligned} \quad (8)$$

The first term on the RHS of Equation 8 can be further simplified using the divergence theorem to arrive at the final form

$$\begin{aligned} \int_\Omega \nabla \times (\mu^{-1} \nabla \times \mathbf{E}) \cdot \nu \; d\Omega = & \int_\Omega (\mu^{-1} \nabla \times \mathbf{E}) \cdot (\nabla \times \nu) \; d\Omega \\ & + \int_{\partial\Omega} \nu \cdot \left[\mathbf{n} \times (\mu^{-1} \nabla \times \mathbf{E}) \right] \; d\Gamma. \end{aligned} \quad (9)$$

The natural boundary condition Eq. 3 is solved automatically resulting in a further simplification

$$\int_\Omega \nabla \times (\mu^{-1} \nabla \times \mathbf{E}) \cdot \nu \; d\Omega = \int_\Omega (\mu^{-1} \nabla \times \mathbf{E}) \cdot (\nabla \times \nu) \; d\Omega. \quad (10)$$

This is the weak formulation and the true solution is approximated as a linear combination of a set of finite element basis functions ψ_i. For simplicity, I'll assume $\psi_i = \nu_i$.

$$\mathbf{E} \approx \sum_i \mathbf{E}_i \nu_i \quad (11)$$

Putting all the pieces together, we arrive at the following set of discrete equations

$$\sum_i \mathbf{E_i} \left[\int_\Omega \mu^{-1} (\nabla \times \nu) \cdot (\nabla \times \nu) \; d\Omega + \int_\Omega i\omega\sigma \nu_i \cdot \nu_j \; d\Omega - \int_\Omega \omega^2 \epsilon \nu_i \cdot \nu_j \; d\Omega \right] = \mathbf{b}_i \quad (12)$$

where $\mathbf{b}_i$ is the contribution of the boundary terms. This can now be assembled in to a matrix vector product of the form $A\mathbf{x} = \mathbf{b}$.

2 Implementation in Palace

The system matrix in Palace is represented as $A = a_0 K + a_1 C + a_2 (M_R + i M_I)$ where K, C and M are the stiffness, damping and the mass matrices. These are defined as

$$K = \int_\Omega \mu^{-1}(\nabla \times \nu) \cdot (\nabla \times \nu)\ d\Omega \tag{13}$$

$$C = \int_\Omega \sigma \nu_i \cdot \nu_j\ d\Omega \tag{14}$$

$$M = \int_\Omega \epsilon \nu_i \cdot \nu_j\ d\Omega \tag{15}$$

with $a_0 = 1$, $a_1 = i\omega$ and $a_2 = -\omega^2$. The mass matrix has both the real and imaginary components due to the complex permittivity.

Now since A is complex valued it can be decomposed into its real part $A_R = K - \omega^2 M_R$ and imaginary part $A_I = C - \omega^2 M_I$ resulting in the following 2×2 matrix

$$A = \begin{bmatrix} A_R & -A_I \\ A_I & A_R \end{bmatrix} \tag{16}$$

Following the notation used in Palace, the system can be written as

$$\begin{bmatrix} A_R \\ A_I \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} K \\ 0 \end{bmatrix} + \begin{bmatrix} 0 & -i\omega \\ i\omega & 0 \end{bmatrix} \begin{bmatrix} C \\ 0 \end{bmatrix} + \begin{bmatrix} -\omega^2 & 0 \\ 0 & -\omega^2 \end{bmatrix} \begin{bmatrix} M_R \\ M_I \end{bmatrix} \tag{17}$$

2.1 Proposed Changes

To model materials with dielectric loss, μ has to be a complex-valued parameter $\mu = \mu_R + i\mu_I$. The inverse of relative permeability is now given by

$$\mu^{-1} = \frac{1}{|\mu|^2}(\mu_R - i\mu_I), \text{ where } |\mu|^2 = (\mu_R^2 + \mu_I^2). \tag{18}$$

The resulting real and imaginary components of the stiffness matrices are

$$K_R = \frac{1}{|\mu|^2} \int_\Omega \mu_R^{-1}(\nabla \times \nu) \cdot (\nabla \times \nu)\ d\Omega \tag{19}$$

$$K_I = -\frac{1}{|\mu|^2} \int_\Omega \mu_I^{-1}(\nabla \times \nu) \cdot (\nabla \times \nu)\ d\Omega. \tag{20}$$

Consequently, the modified system matrix is now composed of $A_R = K_R - \omega^2 M_R$ and $A_I = K_I + C - \omega^2 M_I$.

$$\begin{bmatrix} A_R \\ A_I \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} K_R \\ K_I \end{bmatrix} + \begin{bmatrix} 0 & -i\omega \\ i\omega & 0 \end{bmatrix} \begin{bmatrix} C \\ 0 \end{bmatrix} + \begin{bmatrix} -\omega^2 & 0 \\ 0 & -\omega^2 \end{bmatrix} \begin{bmatrix} M_R \\ M_I \end{bmatrix} \tag{21}$$

Furthermore, the preconditioner system matrix is real-valued so, the new matrix is defined as

$$P = a_0|K_R + iK_I| + a_1 C + a_2|M_R + iM_I|. \tag{22}$$

The following modifications are proposed to the code:

- To keep it consistent with existing framework for permittivity, the magnetic tangent loss will be defined using a new keyword `LossTanMagnetic`.
- Calculate `mat_muinv_imag` and `mat_mu_abs` from `mat_muinv_real` and `LossTanMagnetic`
- Add the following new functions in `GetStiffnessMatrix(K)`
  1. `AddRealStiffnessCoefficients(1.0,mat_mu_real/mat_mu_abs**2)`
  2. `AddImagStiffnessCoefficients(1.0,-mat_mu_inv/mat_mu_abs**2)`
  3. `kr=AssembleOperator()`, `ki=AssembleOperator()`
  4. `M=ComplexParOperator(kr,ki)`, `M=ParOperator(kr)`

2.2 To do

1. Handle BCs: Robin, Numerical wave port, Absorbing and radiation