Sparse computational formulation of dual bounds based on Maxwell Operator

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1 Original Formulation with Explicit Green's Function

In the original formulation, the primal optimization is over polarization currents represented by the image of the source under the $\mathbb{T}$ operator $|\mathbf{T}\rangle = \mathbb{T}\,|\mathbf{S}\rangle$. The fundamental scattering relation is

$$\mathbb{I}_d = \mathbb{I}_d(\mathbb{V}^{-1} - \mathbb{G}_{dd})\mathbb{T} \tag{1}$$

where $\mathbb{I}_d$ is the spatial projection onto the design region, $\mathbb{V}^{-1} = \chi^{-1}\mathbb{I}_d$, and $\mathbb{G}_{dd}$ is the Green's function restricted to the design domain. This can be generalized with the additional application an arbitrary operator $\mathbb{P}$ that commutes with $\mathbb{I}_d$:

$$\mathbb{P} = \mathbb{I}_d(\mathbb{P}\mathbb{V}^{-1} - \mathbb{P}\mathbb{G}_{dd})\mathbb{T} \tag{2}$$

In practice $\mathbb{P}$ is often a spatial projection into a subregion of the entire design region. From this we can formulate scalar constraints of the form

$$\langle\mathbf{S}|\,\mathbb{P}^{\dagger}\,|\mathbf{T}\rangle - \langle\mathbf{T}|\,(\mathbb{V}^{-1}\mathbb{P}^{\dagger} - \mathbb{G}_{dd}\mathbb{P}^{\dagger})\,|\mathbf{T}\rangle = 0 \tag{3}$$

2 Sparse Formulation with Maxwell Operator

The drawback to the original formulation is that $\mathbb{G}_{dd}$ is a dense matrix using a localize spatial basis representation, e.g., a finite difference grid. This leads poor scaling of dual optimization calculations with problem size. Noting that the inverse of the Green's function is proportional to the Maxwell operator $\mathcal{M} = (\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times) - \epsilon_0\omega^2/c^2$, which is sparse under a localized spatial basis, we would like to reformulate the numerics based on $\mathcal{M}$.

By pull out factors of G_{dd} we can rewrite (2) as

$$\mathbb{G}_{dd}^{\dagger}\mathbb{G}_{dd}^{\dagger-1}\mathbb{P} = \mathbb{I}_d\mathbb{G}_{dd}^{\dagger}(\mathbb{G}_{dd}^{\dagger-1}\mathbb{P}\mathbb{V}^{-1}\mathbb{G}_{dd}^{-1} - \mathbb{G}_{dd}^{\dagger-1}\mathbb{P})\mathbb{G}_{dd}\mathbb{T} \tag{4}$$

leading to scalar constraints of the form

$$\langle\mathbf{S}|\,\mathbb{P}^{\dagger}\mathbb{G}_{dd}^{-1}(\mathbb{G}_{dd}\,|\mathbf{T}\rangle) - (\langle\mathbf{T}|\,\mathbb{G}_{dd}^{\dagger})(\mathbb{G}_{dd}^{\dagger-1}\mathbb{V}^{\dagger-1}\mathbb{P}^{\dagger}\mathbb{G}_{dd}^{-1} - \mathbb{P}^{\dagger}\mathbb{G}_{dd}^{-1})(\mathbb{G}_{dd}\,|\mathbf{T}\rangle) \tag{5}$$

We can now declare that $\mathbb{G}_{dd}\,|\mathbf{T}\rangle$ will henceforth be our primal optimization variable. Now the dual optimization involves matrices composed of just $\mathbb{V}$, $\mathbb{G}_{dd}^{-1}$, and diagonal projections $\mathbb{P}$ which are all sparse, allowing for much better problem scaling.

2.1 Computing $\mathbb{G}_{dd}^{-1}$

From the basic relations $\mathcal{M}\mathbf{E} = i\omega\mathbf{J}$ and $\mathbf{E} = (iZ/k)\mathbb{G}\mathbf{J}$ we have

$$\mathcal{M}\mathbb{G} = (k^2/\mu_0)\mathbb{I} \tag{6}$$

where the un-subscripted operators are over all space. We divide space into the design region and background region, delimited by d and b subscripts, respectively.

$$\mathbb{G} = \frac{k^2}{\mu_0}\mathcal{M}^{-1} = \frac{k^2}{\mu_0}\begin{bmatrix} \mathcal{M}_{bb} & \mathcal{M}_{bd} \\ \mathcal{M}_{db} & \mathcal{M}_{dd} \end{bmatrix}^{-1} \tag{7}$$

and making use of the block matrix inversion formula

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix}^{-1} = \begin{bmatrix} A^{-1} + A^{-1}B(D - CA^{-1}B)^{-1}CA^{-1} & -A^{-1}B(D - CA^{-1}B)^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{bmatrix} \tag{8}$$

we have

$$\begin{aligned} G_{dd} &= \frac{k^2}{\mu_0}(\mathcal{M}_{dd} - \mathcal{M}_{db}\mathcal{M}_{bb}^{-1}\mathcal{M}_{bd})^{-1} \\ G_{dd}^{-1} &= \frac{\mu_0}{k^2}(\mathcal{M}_{dd} - \mathcal{M}_{db}\mathcal{M}_{bb}^{-1}\mathcal{M}_{bd}) \end{aligned} \tag{9}$$

In practice the background parts of $\mathcal{M}$ contain the boundary settings for the computational space, e.g., periodic boundary conditions or PML. For a spatially localized representation both $\mathcal{M}_{dd}$ and $\mathcal{M}_{db}\mathcal{M}_{bb}^{-1}\mathcal{M}_{bd}$ are sparse.