FAST CALCULATION OF DIFFRACTION BY PHOTOMASKS

By

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1 Introduction

This work is motivated by the problems of manufacturing and quality control of integrated circuits. Integrated circuits are manufactured by optical lithography. This process involves several steps. First a photomask pattern is designed. The photomask consists of thin films deposited on a thick glass substrate. The photomask pattern is etched into the thin films, or into the glass substrate,
by electron-beam lithography. A photomask is used to pattern one layer or part of one layer of an integrated circuit by optical lithography. Light transmitted through or reflected off the photomask is imaged onto a photoresist film coated on a semiconductor wafer. The pattern on the photoresist is then etched into the wafer by plasma etching. One wafer makes hundreds of copies of an integrated circuit. A schematic diagram of this process is presented in Figure 1.

Simulation of this process has three components. The propagation of a laser pulse from the source to the photomask, the calculation of the near field after passing through the photomask, and the propagation of the scattered field from the photomask to the device. The first and third components of this process are easily and efficiently modeled by Fourier Optics. What we say is efficiently computed takes in excess of 100,000 CPU-hours for the design of a single chip. The scattering problem, i.e. the calculation of the near-field after passing through the photomask, is significantly more computationally intensive. Therefore it is not rigorously solved except for negligibly small fractions of the integrated circuit. To optimize the design of the entire photomask, the near field is obtained from approximations and empirical models with adjustable parameters. The adjustable parameters are calibrated to minimize the difference between experiments and simulations. These expediencies limit the accuracy in the state of the art. Figure 2 diagrams the different components of a full model for optical lithography.

We are interested in the efficient calculation of the near-field as the light passes through the photomask. Efficient simulation of the near-field is necessary for quality control of the production of the photomask, as well as in the optimization process of the design of photomasks for new chips.

The near-field in this problem is modeled by the time-harmonic Maxwell equations, posed in
Figure 2: Schematic diagram of the components in simulating the optical lithography process.

a large 3-dimensional domain with heterogeneous coefficients varying according to the layers and etching in the photomask. Simulation of this problem is computationally intensive due to the size of the problem, and additional difficulties arise in discontinuous material parameters at layer interfaces.

Our work has two main components. First, we develop software to simulate the 3d time-harmonic Maxwell's equations with a perfectly matched layer (PML) in the z-direction using the finite difference frequency domain approach (FDFD). This is a considerable undertaking, and our results with the PML are promising. We explore questions of condition number for various presentations of the Maxwell system discretized by the FDFD method, and note poor convergence properties for well-established iterative schemes such as the generalized minimal residual method (GMRES).

Secondly, we attack this problem by modern, advanced numerical techniques, while using, as a starting point, the Kirchoff approximation. The Kirchoff approximation is an inaccurate but $O(N)$ complexity approximation to the computation of the near-field. While this approximation is inaccurate, we attempt to use the Kirchoff approximation as a starting point for iterative techniques applied to the time-harmonic Maxwell's equations. In particular, we attack the problem with domain decomposition.

Domain decomposition has been applied successfully to many problems in scientific computing with the goals of (i) parallelism and high performance computing, and (ii) robust solution of multiphysics and multiscale problems with interfaces. We were led to this class of methods by the fact that our problem has interfaces with discontinuous data, as well as the need for fast computation. We explored the class of methods known as iterative substructuring methods, and specifically, the Neumann-Neumann type methods. We discover that this class of method is not appropriate for our problem. We describe slow convergence properties and provide a possible explanation of the poor
performance due to lack of coercitivity of the appropriate operators stemming from the Maxwell system in this context. Additionally we provide reference to Schwarz and Robin type domain decomposition techniques that others have successfully applied to FEM discretizations of the Maxwell system.

2 Model

2.1 Time-Harmonic Maxwell’s Equations and Boundary Conditions

The EM scattering problem in optical lithography is modeled by the time-harmonic Maxwell’s equations. We will consider the model after normalization, which is detailed in the Appendix. These are given by,

\begin{align}
  i \mu_r H &= \nabla \times E + f^h, \\
  -i \epsilon_r E &= \nabla \times H + f^e, \\
\end{align}

along with appropriate boundary conditions. Here \( E \) denotes the electric field, \( H \) the magnetic field, \( \epsilon_r \) is the relative electric permittivity, and \( \mu_r \) is the relative magnetic permittivity. We include forcing terms \( f^h \) and \( f^e \) to model the incident field caused by a laser pulse before the scatterers (etched regions) are introduced.

For proof-of-concept, we pose the problem of determining the solution of Equations (1) and (2) in a 3d computational domain that captures the essential features of the photomask, with appropriate boundary conditions. The computational domain is shown in Figure 3. The domain is layered in the \( z \)-direction consisting of materials with different permittivities, and etching creates changes in permittivity in the \( x \) - and \( y \) -directions. We assume the geometry is such that the permittivity is constant on polygonal sections with edges in coordinate directions. Thus the permittivities are given by diagonal matrices.

The photomask is very large (5 \( \times \) \( 10^5 \) wavelengths) in \( x \) - and \( y \) -directions. Taking the entire photomask as one computation domain is not possible. Therefore, we break up the computation domain into managable pieces to solve Maxwell’s Equations. The dependence of the near-field on the photomask is approximately local: the near-field at a point \( A \) is not significantly affected by parts of the mask that are 5 wavelengths or more distant to point \( A \). Any boundary conditions imposed at the \( x \) and \( y \) boundaries of the computation domain are artificial. They don’t represent the correct physics of the problem. We use periodic boundary conditions for simplicity. The solution is valid in a central part of the computation domain, away from \( x \) and \( y \) boundaries, if the computation domain is large enough (on the order of 5 wavelengths or more in \( x \) and \( y \)-directions). Some circuits such as memory arrays are periodic. In such cases, the actual period of the circuit is used and the solution is valid in the entire computation domain.

In the positive and negative \( z \)-directions, we must simulate homogeneous media extending to infinity. When truncating the domain, we require a treatment of these boundaries that does not introduce nonphysical reflections of the outgoing scattered field back into the region of interest. This may be achieved in one of a few ways. We accomplish this by the use of a perfectly matched layer (PML).
2.2 Perfectly Matched Layer

A perfectly matched layer (PML) is employed by padding the computational domain along the non-reflecting boundary. The PML technique was first introduced in [3]. The uniaxial PML formulation soon followed in [11], and the two were shown to be equivalent. We use the uniaxial PML here.

The non-reflecting condition is achieved by designing an artificial anisotropic material within the PML region that does not reflect waves. The PML is also designed to damp the waves that enter into it by an exponential factor. Thus, by the time an outgoing wave has passed through the PML and reaches the exterior boundary, it has decayed to be nearly 0. Here, then, a homogeneous Dirichlet boundary condition may be used. The only waves reaching the Dirichlet boundary (that is, the only waves that will be reflected back towards the region of interest) have already been almost entirely attenuated by the PML, and cause very little error in the solution. The PML for our geometry is illustrated in Figure 3.

The material parameters specified within the PML are $\bar{\epsilon} = \epsilon_r \bar{S}$ and $\bar{\mu} = \mu_r \bar{S}$, where

$$\bar{S} = \begin{bmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & 1 / s \end{bmatrix}.$$ 

For the continuous problem, in theory, the PML will be non-reflecting for any $s$, regardless of the outgoing wave’s frequency and angle of incidence. When discretizing using finite differences, however, we must take care to avoid discontinuous material parameters that would introduce errors. Also, we must ensure that the waves transmitted into the PML are rapidly attenuated. With this in mind, we choose

$$\bar{S} = \begin{bmatrix} 1 + \frac{ia}{\epsilon_r} & 0 & 0 \\ 0 & 1 + \frac{ia}{\epsilon_r} & 0 \\ 0 & 0 & \frac{1}{1 + \frac{ia}{\mu_r}} \end{bmatrix},$$

where the dimensionless function $\sigma(z)$ is zero at the PML interface and increases as $z$ approaches the boundary. At the interface between the domain of interest and the PML, then, $\bar{S}$ is the identity, ensuring the continuity of $\epsilon_r$ and $\mu_r$. Furthermore, the transmitted fields acquire a factor of $e^{-\sigma \sqrt{\frac{\mu_r}{\epsilon_r} \cos(\theta)} (z - z_0)}$, where $z_0$ denotes the location of the PML boundary. Thus, the waves are attenuated, especially as they approach the exterior boundary where $\sigma$ is larger. The attenuation depends on the angle of incidence. Maximum attenuation is achieved for waves incident in the normal direction, while waves that graze the PML interface will not be attenuated as much.

3 Kirchhoff’s Approximation

In the late 1800s Gustav Kirchhoff studied light diffraction by an aperture in an opaque screen. Kirchhoff devised an approximation of the near-field that allows for a computation of $O(N)$ complexity. This efficiency is obtained by ignoring the aperture next to the screen, and ignoring the screen next to the aperture. Once the near-field is approximated in a plane, it is easily propagated to the image plane using Green’s Theorem. Figure 4 illustrates this idea.
Figure 3: Domain of interest padded with a Perfectly Matched Layer.

Figure 4: Illustration of Kirchoff approximation.
Clearly this approximation ignores essential physics if one is greatly concerned with accuracy. Thus various improvements have been made. However, these improvements are still inaccurate, and the explicit computation of the time-harmonic Maxwell’s equations would provide a better solution.

4 Finite Difference Frequency Domain

4.1 Forcing Term Expressed as Deviation from a Background

The electromagnetic field \((E, H)\) is sourced by the electric and magnetic current densities \(J, M\). Frequently the original source of the EM radiation is far from the computation domain. For example the laser that illuminates a lithographic photomask is far from the photomask and there are many optical components in between. In such cases, expressing the forcing function in terms of a known incident wave is advantageous. We introduce the concepts of background geometry, materials and fields. The background problem has three properties: it is easy to solve; it has the same primary sources as in the original problem; and the background geometry and materials agree with those in the original problem in most places. The original problem is:

\[
\nabla \times E = i\mu_r H + M_{pri} \\
\nabla \times H = -i\epsilon_r E + J_{pri}
\]

where \(\mu_r\) and \(\epsilon_r\) are inhomogeneous and possibly anisotropic. The background problem is:

\[
\nabla \times E_{bg} = i\mu_{bg} H_{bg} + M_{pri} \\
\nabla \times H_{bg} = -i\epsilon_{bg} E_{bg} + J_{pri}
\]

We difference the above equations to obtain:

\[
\nabla \times (E - E_{bg}) = i\mu_r (H - H_{bg}) + i(\mu_r - \mu_{bg}) H_{bg} \\
\nabla \times (H - H_{bg}) = -i\epsilon_r (E - E_{bg}) - i(\epsilon_r - \epsilon_{bg}) E_{bg}
\]

We define the scattered field as the difference between the fields of the original problem and the background fields:

\[
E_{sca} = E - E_{bg} \\
H_{sca} = H - H_{bg}
\]

We define the induced magnetic and electric current densities:

\[
M_{ind} = i(\mu_r - \mu_{bg}) H_{bg} \\
J_{ind} = -i(\epsilon_r - \epsilon_{bg}) E_{bg}
\]
The induced currents exist only where the background materials differ from the materials of the original problem. Maxwell’s equations for the scattered fields are:

\[
\nabla \times E_{\text{sca}} = i\mu_r H_{\text{sca}} + M_{\text{ind}} \quad (18)
\]

\[
\nabla \times H_{\text{sca}} = -i\epsilon_r E_{\text{sca}} + J_{\text{ind}} \quad (19)
\]

The scattered field satisfies the original PDE but with a different forcing function. The scattered fields are excited by the induced electric current density \(J_{\text{ind}}\) and the induced magnetic current density \(M_{\text{ind}}\).

**4.2 Setting up FDFD Equations**

We discretize the time-harmonic Maxwell’s equations:

\[
\nabla \times E_{\text{sca}} = i\mu_r H_{\text{sca}} + M_{\text{ind}} \quad (21)
\]

\[
\nabla \times H_{\text{sca}} = -i\epsilon_r E_{\text{sca}} + J_{\text{ind}} \quad (22)
\]

(23)

using Yee’s grid [Kane S. Yee, “Numerical Solution of Initial Boundary Value Problems Involving Maxwell’s Equations in Isotropic Media,” IEEE Trans. Antennas and Propagation, Vol. AP-14, No. 3, pp. 302-307, May 1966]. The discretized equations form a linear system of equations. There are at least three ways to set up the linear system of equations. We can eliminate the magnetic or the electric field from the vector of unknowns. Then we have \(3N_xN_yN_z\) complex, scalar unknowns where \(N_xN_yN_z\) is the number of Yee cells in the computation domain. Alternatively, we can have \(6N_xN_yN_z\) complex, scalar unknowns which are the electric and magnetic vector field components; and solve a first-order difference equation.

**4.3 Electric Field FDFD Equation**

We eliminate the magnetic field and set up a linear system of equations for the electric field. The action of the coefficient matrix on the unknown vector \(E\) is calculated as follows:

\[
A_e E_{\text{sca}} = -i\nabla_h \times \left(\mu_r^{-1}\nabla_e \times E_{\text{sca}}\right) + i\epsilon_r E_{\text{sca}}
\]

The finite-difference curl operators \(\nabla_e\) and \(\nabla_h\) are different because they act on staggered grids. These operators particularly differ at the boundary of the computation domain. The forcing term for the electric field FDFD equations is:

\[
f_e = J_{\text{ind}} - i\nabla_h \times \left(\mu_r^{-1}M_{\text{ind}}\right)
\]

We obtain the electric field by solving the equation:

\[
A_e E_{\text{sca}} = f_e
\]

and calculate the total field: \(E = E_{\text{sca}} + E_{\text{bg}}\). The magnetic field is obtained from the electric field:

\[
H = -i\mu_r^{-1}\nabla_e \times E
\]

In the last equation we assumed that the magnetic current source of the original problem \(M_{\text{ori}}\) is zero in the computation domain.
4.4 Magnetic Field FDFD Equation

We eliminate the electric field to set up a linear system of equations for the magnetic field. The action of the coefficient matrix on the unknown vector $H$ is calculated as follows:

$$A_h H_{sca} = i\nabla_e \times (\epsilon^{-1} \nabla_h \times H_{sca}) - i\mu_r H_{sca}$$

The forcing term for the magnetic field FDFD equations is:

$$f_h = M_{ind} + i\nabla_e \times (\epsilon^{-1} J_{ind})$$

We obtain the magnetic field by solving the equation:

$$A_h H_{sca} = f_h$$

and calculate the total field: $H = H_{sca} + H_{bg}$ The electric field is obtained from the magnetic field:

$$E = i\epsilon^{-1} \nabla_h \times H$$

In the last equation we assumed that the electric current source of the original problem $J_{ori}$ is zero in the computation domain.

4.5 First-Order FDFD Equation

In this case we choose the unknown vector $[E, H]$. We don’t eliminate either $E$ or $H$. This results in an equation that has only first order derivatives. We solve the linear equation:

$$A \begin{bmatrix} E \\ H \end{bmatrix} = f$$

The matrix-vector product is calculated as:

$$A \begin{bmatrix} E \\ H \end{bmatrix} = \begin{bmatrix} \nabla_e \times E - i\mu_r H \\ -i\epsilon E + \nabla_h \times H \end{bmatrix}$$

The forcing term is:

$$f = \begin{bmatrix} M_{ind} \\ J_{ind} \end{bmatrix}$$

4.6 Performance of the Perfectly Matched Layer

The PML described in Section 2.2 worked as expected. Figure 5 shows the errors in the $y$-component of the scattered $E$ field computed using the first-order FDFD formulation, both with and without a PML. It is clear that, without a PML, undesirable reflections are causing large errors throughout the domain. With the use of the PML, however, errors are small within the domain of interest. We are not concerned with error in the PML layer itself, since we do not need to obtain field values there.
4.7 Condition Number of Equations

We initially coded the linear equations without storing the coefficient matrices. We evaluated the matrix-product by evaluating finite-difference curls according to Yee’s grid. We found that GMRES reduced the residual slowly and stalled. To investigate the cause, we formed the sparse matrices for a small problem (1 wavelength x 1 wavelength x 3.5 wavelength) and solved the linear equations with MATLAB back slash operation and estimated the condition numbers. We observed the following performance:

<table>
<thead>
<tr>
<th>Unknown Vector</th>
<th># Unknowns</th>
<th>Condition Number</th>
<th>Relative Residual after 100 GMRES Iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E$</td>
<td>10500</td>
<td>23400</td>
<td>0.29</td>
</tr>
<tr>
<td>$H$</td>
<td>10500</td>
<td>15500</td>
<td>0.13</td>
</tr>
<tr>
<td>$[E, H]$</td>
<td>31500</td>
<td>4400</td>
<td>0.87</td>
</tr>
</tbody>
</table>

The first-order equation had the lowest condition number, yet it had the largest GMRES relative residual. GMRES was run for 100 iterations without restarting. Restarting did not reduce the residual.

The fields computed by the three formulations agree when the linear equations are solved without using an iterative solver. This can be seen in the figures below.

5 Domain Decomposition

Domain decomposition (DDM) techniques for partial differential equations attempt to solve independent subdomain problems, rather than the problem as originally posed on the full domain. These methods have been designed with two primary purposes in mind. Originally, domain decomposition was developed as a methodology of parallelism for large, out-of-core problems. There exists a library of literature in this context from mathematicians, computer scientists, and computational
Figure 6: Coefficient matrix for a 3-D FDFD E-field equation

Figure 7: Coefficient matrix for a 3-D FDFD H-field equation

In more recent years, DDM has received growing interest as a tool for handling multi-physics problems where material parameters or physical models vary between physical subdomains, as well as for problems with multi-scale phenomena characterized by interfaces. In this context DDM has been successfully applied to problems of fluid flow [12], the coupling of Darcy and Stokes flows [7], [8], as well as in problems of electrostatics [10], [5], among other applications.

The physical problem we are interested in computing is composed of layered materials separated by interfaces. This combined with the size of the problem suggests the use of domain decomposition techniques.

In recent years there has been a growing interest in domain decomposition for the time-harmonic Maxwell’s equations. Methods of iterative substructuring type [1], [2] have been developed using
complicated Robin type transmission conditions, as well as Schwarz type preconditioners [18]. In this work, we attempt to develop an iterative substructuring algorithm of Neumann-Neumann type. Neumann-Neumann methods have the advantage of employing non-overlapping subdomains and obtaining convergence independent of the resolution. That is, the Neumann-Neumann method has $O(1)$ complexity. Thus the computational complexity of a computational paradigm employing Neumann-Neumann methods is determined entirely by the complexity of the subdomain solvers, while simultaneously reducing the size of $N$ for these solvers and allowing parallelism. Additionally, due to their popularity, Neumann-Neumann type methods have been extensively researched, and it is well-understood how to obtain good scaling properties with many domains through the use of some sort of global correction, e.g. a Balancing Neumann-Neumann method. Neumann-Neumann type methods have also been developed for unusual interface behavior in problems with multiscale phenomena characterized by interfaces. We note, however, that the method developed here demonstrated extraordinarily slow convergence in a 3d simulation using finite-difference frequency domain discretizations for the subdomain problems. Insight into why this is the case may be found in [9], where it is explained that, in general, classical iterative methods (e.g. Krylov methods, domain decomposition methods, and multigrid) have tremendous difficulty with rate of convergence on the Helmholtz problem. Since the 2D Helmholtz problem can be considered as a special case of the time-harmonic Maxwell system, the difficulties presented in [9] may apply to our problem. This suggests the need for more research and the development of methods to accelerate convergence for domain decomposition schemes and other iterative methods applied to the time-harmonic Maxwell system.

Iterative substructuring algorithms of Neumann-Neumann type work by first defining a multi-domain formulation of a model partial differential equation problem. An equation posed on the interface is then developed whose solution will guarantee that the multidomain formulation is consistent with the original partial differential equation. An iterative procedure is then performed to solve the interface equation and the independent subdomain problems.
5.1 Two-domain time harmonic Maxwell’s equations

In this section we develop the two-domain model. This is trivially extended to the many subdomain model by requiring the transmission conditions obtained here hold between all adjacent subdomains.

Rather than solving the problem on the domain $\Omega$, we subdivide the domain into two components $\Omega_1$ and $\Omega_2$ such that $\cap_i \Omega_i = \emptyset$, $\cup_i \Omega_i = \Omega$, and $\cap_i \overline{\Omega_i} := \Gamma$ is an 2 dimensional manifold.

Then we consider the two-domain formulation of the time harmonic Maxwell system given by,

Subdomain problems:

\[
\begin{align*}
&\mu_r H_i = \nabla \times E_i + f^h, \quad \text{in } \Omega_i, i = 1, 2, \\
&-\epsilon_r E_i = \nabla \times H_i + f^e, \quad \text{in } \Omega_i, i = 1, 2.
\end{align*}
\]  

Transmission conditions:

\[
\begin{align*}
(n \times E_1)|\Gamma = (n \times E_2)|\Gamma, \\
(n \times \text{curl } E_1)|\Gamma = (n \times \text{curl } E_2)|\Gamma.
\end{align*}
\]  

The first of these transmission conditions ensures that the tangential component of the electric field is continuous across the interface $\Gamma$, while the second of these transmission conditions ensures that the tangential component of the magnetic field is continuous across the interface $\Gamma$.

It is a well-known result that these transmission conditions ensure that a solution to the two-domain problem solves the single domain problem [2].

5.2 Independent Subdomain Problems & Steklov-Poincaré Interface Equation

Clearly the problem given by (24)-(25) does not consist of independent subdomain problems, as the transmission conditions (25) couple the solutions of the two subdomain problems. Thus we would like to solve instead the decoupled problems,

\[
\begin{align*}
&i\mu_r H_i = \nabla \times E_i + f^h, \quad \text{in } \Omega_i, \\
&-i\epsilon_r E_i = \nabla \times H_i + f^e, \quad \text{in } \Omega_i, \\
&(n^i \times E_i)|\Gamma = \lambda,
\end{align*}
\]  

for some value $\lambda$ to be determined. For any value of $\lambda$, we satisfy the first transmission condition

\[
(n \times E_1)|\Gamma = (n \times E_2)|\Gamma,
\]

however, we have no reason to expect that this problem ensures continuity of the tangential component of the magnetic field. Thus we must develop a tool for finding the correct $\lambda$ such that

\[
(n \times \text{curl } E_1)|\Gamma = (n \times \text{curl } E_2)|\Gamma
\]

is satisfied.

Applying superposition, we define $E_i^\lambda$ and $E_i^f$ to be the responses to the interface data $\lambda$ and or forcing term $f$. Thus, these terms solve the equations,

\[
\begin{align*}
&\nabla \times (\mu_r^{-1} \nabla \times E_i^\lambda) - \epsilon_r E_i^\lambda = 0 \quad \text{in } \Omega_i, \\
&(n^i \times E_i^\lambda) = \lambda \quad \text{on } \Gamma, \\
&i\mu_r H_i = \nabla \times E_i^f + f^h \quad \text{in } \Omega_i, \\
&-i\epsilon_r E_i^f = \nabla \times H_i + f^e \quad \text{in } \Omega_i, \\
&(n^i \times E_i)|\Gamma = 0,
\end{align*}
\]  

\(13\)
respectively.

Then we define the operators

\[ S\lambda := (\mathbf{n} \times \text{curl} \, E^2_\lambda)|_\Gamma - (\mathbf{n} \times \text{curl} \, E^1_\lambda)|_\Gamma, \] (31)

\[ \chi := (\mathbf{n} \times \text{curl} \, E^f_1)|_\Gamma - (\mathbf{n} \times \text{curl} \, E^f_2)|_\Gamma, \] (32)

and seek to solve

\[ S\lambda = \chi. \] (33)

It is an exercise in algebra to see that if \( \lambda \) satisfies this Steklov-Poincaré equation, then a solution to the independent subdomain problems will solve the two-domain formulation of the time-harmonic Maxwell system, and thus solves the original problem.

### 5.3 Algorithm nnMaxwell

An algorithm of the Neumann-Neumann type for this problem has the following form:

Given \( \lambda^0 \),

1. Solve

\[
\begin{aligned}
    i\mu_{r,i} H^{n+1}_i &= \nabla \times E^{n+1}_i + f^h \quad \text{in } \Omega_i, \\
    -i\epsilon_{r,i} E^{n+1}_i &= \nabla \times H^{n+1}_i + f^e \quad \text{in } \Omega_i, \\
    (\mathbf{n} \times E^{n+1}_i) &= \lambda^n \quad \text{on } \Gamma.
\end{aligned}
\] (34)

2. Then solve the auxiliary problem,

\[
\begin{aligned}
    \nabla \times (\mu_{r,i}^{-1} \nabla \times \Psi^{n+1}_i) - \epsilon_{r,i} \Psi^{n+1}_i &= 0 \quad \text{in } \Omega_i, \\
    (\mathbf{n} \times \text{curl} \, \Psi^{n+1}_i) &= [\mathbf{n} \times \text{curl} \, E^{n+1}_i]|_\Gamma \quad \text{on } \Gamma.
\end{aligned}
\] (35)

3. Then update \( \lambda \),

\[ \lambda^{n+1} = \lambda^n - \theta [\Psi^{n+1}] |_\Gamma. \] (36)

4. Check stopping criteria, e.g. \( \|([\mathbf{n} \times \text{curl} \, E])|_\Gamma \| \), return to (1) if criteria is not met, else exit.

We note that the performance of this algorithm was extremely poor, exhibiting pathological dependence on the parameter \( \theta \), and excruciatingly slow convergence when \( \theta \) was chosen carefully. In the next section, we show that this algorithm is equivalent to a Richardson scheme for the interface equations \( S\lambda = \chi \), and suggest an explanation for its poor performance by examining the properties of the weak characterization of the operator \( S \).
5.4 Richardson Scheme

It is helpful to notice that this algorithm is a pre-conditioned Richardson scheme for the equation $S\lambda = 0$. To see this, notice,

$$
\Psi_1^{n+1} = S_1^{-1}(S\lambda^n - \chi), \quad (37)
$$
$$
\Psi_2^{n+1} = -S_2^{-1}(S\lambda^n - \chi), \quad (38)
$$

so that we can write the $\lambda$ update step as,

$$
\lambda^{n+1} = \lambda^n - \theta(S_1^{-1} + S_2^{-1})(S\lambda^n - \chi). \quad (39)
$$

5.4.1 Difficulties with Convergence

Typically, a proof of convergence for a Neumann-Neumann type method proceeds as follows:

1. The algorithm is shown to be equivalent to a preconditioned Richardson scheme, using as a preconditioner an operator based on a splitting of the Steklov-Poincaré operator $S$. (Section 5.4)

2. The weak form of the equation $S\lambda = \chi$ is developed.

3. The components $S_i$ are shown to be continuous and coercive on an appropriate space.

4. These properties are used to show that a particular mapping is a contraction on a Hilbert space, and the Banach Contraction Mapping Principle is applied to guarantee convergence.

In our case, the problem with a proof of this kind arises in step (2), as the operator splitting presented here does not result in coercive operators $S_i$ on the appropriate Hilbert space.

First we develop the appropriate spaces. In the following the space $H^s(U)$, $s \in \mathbb{R}$ defines the usual Sobolev space, with norm given by $\| \cdot \|_{s,U}$. Here $U$ is an arbitrary subset $U \in \mathbb{R}^d$ for $d \in \{2, 3\}$. We denote the duality pairing between the spaces $H^s(U)$ and $H^{-s}(U)$ by $\langle \cdot, \cdot \rangle_{s,U}$. Additionally we denote by $H(\text{curl};U)$ and $H(\text{div};U)$ the set of real or complex functions $u \in (L^2(U))^3$ such that curl $u \in (L^2(U))^3$ and $\nabla \cdot u \in L^2(U)$, respectively.

We will need to define the tangential divergence of a tangential vector field $\mu$. Let $\mu \in (H^{-1/2}(\partial \Omega))^3$ with $(\mu \cdot n)|_{\partial \Omega} = 0$. We define the tangential divergence $\text{div}_\tau \mu \in H^{-3/2}(\partial \Omega)$ by

$$
\langle \text{div}_\tau \mu, \eta \rangle_{3/2,\partial \Omega} = -\langle \mu, (\nabla \mathcal{R}_2 \eta)|_{\partial \Omega} \rangle_{1/2,\partial \Omega}, \quad \forall \eta \in H^{3/2}(\partial \Omega),
$$

(40)

where $\mathcal{R}_2$ denotes any continuous extension operator from $H^{3/2}(\partial \Omega)$ into $H^2(\Omega)$.

Now we introduce the Hilbert spaces $X_{\partial \Omega}$ and $X_{\Sigma}$, where $\Sigma \subset \partial \Omega$ denotes a nonempty subset of the boundary:

$$
X_{\partial \Omega} := \{ \mu \in (H^{-1/2}(\partial \Omega))^3 | (\mu \cdot n)|_{\partial \Omega} = 0 \text{ and } \text{div}_\tau \mu \in H^{-1/2}(\partial \Omega) \},
$$

(41)
$$
X_{\Sigma} := \{ \mu \in (H^{-1/2}(\Sigma))^3 | (\mu \cdot n)|_{\Sigma} = 0 \text{ and } \text{div}_\tau \mu \in H^{-1/2}(\partial \Omega) \},
$$

(42)
where $\tilde{\mu}$ denotes the extension by 0 on $\partial \Omega \setminus \Sigma$. We endow these spaces with norms:

$$
\|\mu\|_{X_{\partial \Omega}} := \|\mu\|_{-1/2, \partial \Omega} + \|\text{div}_\tau \mu\|_{-1/2, \partial \Omega}, 
$$

(43)

$$
\|\mu\|_{X_{\Sigma}} := \|\mu\|_{-1/2, \Sigma} + \|\text{div}_\tau \tilde{\mu}\|_{-1/2, \partial \Omega}.
$$

(44)

In [1, 2] it is proven that if $\Omega \in C^{1,1}$ or $\Omega$ is a convex polyhedron, the space $X_{\partial \Omega}$ is the space of tangential traces of $H(\text{curl}; \Omega)$, and $X_{\Sigma}$ is the space of tangential traces of $H_{\partial \Omega \setminus \Sigma}(\text{curl}; \Omega) := \{v \in H(\text{curl}; \Omega) \mid (n \times v)|_{\partial \Omega \setminus \Sigma} = 0\}$. (45)

Additionally it was shown that there exist two linear continuous operators

$$
R_{\partial \Omega} : X_{\partial \Omega} \to H(\text{curl}; \Omega),
$$

(46)

$$
R_{\Sigma} : X_{\Sigma} \to H_{\partial \Omega \setminus \Sigma}(\text{curl}; \Omega)
$$

(47)

satisfying

$$
(n \times R_{\partial \Omega} \mu)|_{\partial \Omega} = \mu, \quad (n \times R_{\Sigma} \mu)|_{\Sigma} = \mu
$$

(48)

for all $\mu \in X_{\partial \Omega}$ or $\mu \in X_{\Sigma}$.

Next we develop the weak form of the operators $S_i$. In the following we assume $\epsilon_i = \mu_i = 1$ for ease of exposition. We denote by $R_{\Gamma,i} : X_{\Gamma} \to H_{\partial \Omega \setminus \Gamma}(\text{curl}; \Omega_i)$ a linear continuous extension operator acting from the interface to subdomain $i$. Then we calculate,

$$
\langle S_\lambda, \mu \rangle = -\sum_{i=1}^{2} \int_{\Gamma} (n^i \times \text{curl} \ E^\lambda_i) \cdot \mu
$$

(49)

$$
= -\sum_{i=1}^{2} \int_{\Gamma} (n^i \times \text{curl} \ E^\lambda_i) \cdot R_{\Gamma,i} \mu
$$

(50)

$$
= -\sum_{i=1}^{2} \int_{\partial \Omega_i} (n^i \times \text{curl} \ E^\lambda_i) \cdot R_{\Gamma,i} \mu
$$

(51)

$$
= \sum_{i=1}^{2} \int_{\Omega_i} \text{curl} \ E^\lambda_i \cdot \text{curl} \ R_{\Gamma,i} \mu - \int_{\Omega_i} \text{curl} \ curl \ E^\lambda_i \cdot R_{\Gamma,i} \mu
$$

(52)

$$
= \sum_{i=1}^{2} \int_{\Omega_i} \text{curl} \ E^\lambda_i \cdot \text{curl} \ R_{\Gamma,i} \mu - \int_{\Omega_i} E^\lambda_i \cdot R_{\Gamma,i} \mu
$$

(53)

Defining the bilinear form

$$
a_i(u, v) := \int_{\Omega_i} \text{curl} \ u \cdot \text{curl} \ v - \int_{\Omega_i} u \cdot v,
$$

(54)

(55)

we note that we have $\langle S_i \lambda, \mu \rangle = a_i(E^\lambda_i, R_{\Gamma,i} \mu)$, which is clearly not a coercive operator due to the 2nd term in $a_i$. 

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6 Conclusion

In this work we develop are concerned with the efficient solution of a 3d electromagnetic scattering problem that arises in the modeling of the optical lithography process used in chip design.

We first develop software for the 3d time-harmonic Maxwell system discretized by the finite difference frequency domain approach, using a perfectly matched layer in the z-direction. We analyze properties of the resulting linear system in the $H$ curl curl framework, $E$ curl curl framework, and in the first order $E - H$ system.

Additionally, we explore the application of iterative domain decomposition techniques to the model, initiated by the Kirchoff approximation. We encounter tremendous difficulties with methods of the Neumann-Neumann type, and explore a possible explanation for this in the lack of coercivity of the components of the Neumann-Neumann type preconditioner for this problem.

A Normalizing Maxwell’s Equations

Time-harmonic form of Maxwell’s Equations are:

$$\nabla \times E = i\omega \mu H + M$$

$$\nabla \times H = -i\omega \varepsilon E + J$$

We obtain these equations from the time-dependent Maxwell’s equations by using the $e^{-i\omega t}$ time dependence, and factoring it out. We will now normalize these equations and render them dimensionless. To this end we first define the relative electric permittivity $\varepsilon_r$ and magnetic permeability $\mu_r$:

$$\varepsilon_r = \varepsilon/\varepsilon_0$$

$$\mu_r = \mu/\mu_0$$

$$\varepsilon_0 = 8.85... \times 10^{-12} \text{ Farad/m}$$

$$\mu_0 = 4\pi \times 10^{-7} \text{ Henry/m.}$$

The constants $\varepsilon_0$ and $\mu_0$ are the electric permittivity and magnetic permeability of vacuum, respectively. Next, we redefine the magnetic field as the magnetic field times the wave impedance of free-space:

$$\tilde{H} = H \sqrt{\mu_0/\varepsilon_0}$$

The units of $\tilde{H}$ and $E$ are the same. We redefine space coordinates as:

$$\tilde{x} = k_0 x$$

$$k_0 = \omega \sqrt{\mu_0 \varepsilon_0}$$
Then Maxwell’s equations become:
\[
\nabla \times E = i\mu_r \tilde{H} + \tilde{M} \\
\nabla \times \tilde{H} = -i\epsilon_r E + \tilde{J}
\]
(66) \hspace{1cm} \hspace{1cm} (67) \hspace{1cm} \hspace{1cm} (68)

We redefined the magnetic and electric current densities as:
\[
\tilde{M} = M/k_0 \\
\tilde{J} = J \sqrt{\mu_0/\epsilon_0}/k_0
\]
(69) \hspace{1cm} \hspace{1cm} (70)

We drop all tilde symbols and obtain:
\[
\nabla \times E = i\mu_r H + M \\
\nabla \times H = -i\epsilon_r E + J
\]
(72) \hspace{1cm} \hspace{1cm} (73) \hspace{1cm} \hspace{1cm} (74)

In the above equation, the units of \(E, H, M\) and \(J\) are the same (Volt/m). Normalizing them by an arbitrary, constant electric field such as 1 V/m renders them dimensionless. Therefore all quantities in the above normalized Maxwell’s equations, including distance, are dimensionless.

References


Figure 9: The real parts of $E_y$ and $H_x$ field components computed by three different FDFD formulations. The relative difference is on the order of 3%. The mesh size is $1/10$ of the vacuum wavelength. Relative difference is the ratio of $\ell_2$ norms.