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# NEW DIRECTIONS IN PHOTONICS SIMULATION: LANCZOS RECURSION AND FINITE-DIFFERENCE TIME-DOMAIN[1]

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## INTRODUCTION

Computational Integrated Photonics (CIP) is the area of computational physics that treats the propagation of light in optical fibers and in integrated optical circuits (the photonic analog of electronic circuits). The purpose of integrated photonics simulation is to develop the computational tools that will support the design of photonic and optoelectronic integrated devices. CIP has, in general, two thrusts: (i) predictive models of photonic device behavior that can be used reliably to enhance significantly the speed with which designs are optimized for development applications, and (ii) to further our ability to describe the linear and nonlinear processes that occur - and can be exploited - in real photonic devices.

Experimental integrated optics has been around for over a decade with much of the work during this period centered on proof-of-principle devices that could be described (generally fit) using simple analytic and numerical models. Recent advances in material (especially semiconductor) growths, photolithography, and device complexity have conspired to reduce significantly the number of devices that can be designed with simple models and to increase dramatically the interest in CIP. In the area of device design, CIP is viewed as critical to understanding device behavior and to optimization. In the area of propagation physics, CIP is an important tool in the study of nonlinear processes in integrated optical devices and fibers. In this talk I will discuss two of the new directions we have been investigating in CIP: Lanczos recursion and finite-difference time-domain.

## LANCZOS RECURSION

The Helmholtz equation plays a central role in the description of propagation phenomena in optics and acoustics. The paraxial approximation to the Helmholtz equation, also known as the paraxial wave equation, has long been the instrument of choice for performing calculations because it is amenable to solution by accurate marching techniques. The generation of accurate solutions to the unapproximated Helmholtz equation by marching, on the other hand, requires the evaluation of a square root operator applied to some initial field. By using an orthogonalization procedure due to Lanczos one can generate a low-dimensional

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representation, valid over a sufficiently short propagation step, which accurately diagonalizes the square root operator.[1-2]

One shortcoming of this Lanczos propagation scheme is that it is restricted to Hermitian operators, which prohibits its use with imaginary refractive indices, representing gain or loss. This restriction excludes a wide class of interesting propagation applications. Even when loss is not explicitly included in the problem, it is customary to include loss in a border region along the grid boundary to prevent power from reflecting from the boundaries back into the interior of the computational grid. We have developed a generalization of the previous Lanczos Helmholtz solver [1-2] that allows general complex refractive index distributions to be considered.

After factoring out a complex monochromatic carrier wave, one can without loss of generality write the Helmholtz equation as

$$\frac{\partial^2\psi}{\partial z^2} + 2ik\frac{\partial\psi}{\partial z} + H\psi = 0\,, \tag{1}$$

where the operator $H$ is defined by

$$H \equiv \nabla_\perp^2 + k^2\left(\frac{n(x,y,z)^2}{n_0^2} - 1\right)\,, \tag{2}$$

and where $n(x,y,z) = n'(x,y,z)[1 + i\delta(x,y,z)]$ is a complex refractive index that varies weakly with $z$. Equation (1) is satisfied by two independent solutions corresponding to waves propagating to the right and to the left. The rightward propagating solution can be written formally as

$$\psi(z) = \exp\left\{-iz\left[k - k(1 + H/k^2)^{1/2}\right]\right\}\psi(0)\,. \tag{3}$$

One can evaluate Eq (3) by introducing a low-dimensional diagonal representation of the operator H. First one constructs a basis from the $N$ Krylov vectors $\psi(0)$, $H\psi(0)$, ..., $HN-1\psi(0)$, where the components of the vectors are the function values on the computational grid, and the second derivatives in $H$ are evaluated by expressing $\psi(0)$ as a finite Fourier series. These vectors are independent but not orthonormal. Since the operator $H$ is nonHermitian, the standard Lanczos orthogonalization procedure [2] is not appropriate for deriving an orthonormal set of vectors from the Krylov vectors. We therefore generalize the standard Lanczos procedure as follows.

We define a set of "right" column vectors $|q_0>$, ..., $|q_{N-1}>$ and a set of "left" row vectors $<q_0'|$, ..., $<q_{N-1}'|$. The orthogonality for the different vectors is defined by the relation

$$<q_n'|q_{n'}> = \delta_{nn'}\,. \tag{4}$$

The left-hand side of Eq. (4) signifies an inner product between $< q'_n|$ and $|q_{n'} >$, where the components of $< q'_n|$ and $|q_n >$ are, in general, not the complex conjugates of each other, as they are when $H$ is Hermitian. The following pair of recursion relations generalizes the standard Lanczos orthogonalization procedure and leads to a symmetric matrix representation of $H$:

$$\beta_n|q_{n+1} > \;=\; H|q_n > \;-\; \alpha_n|q_n > \;-\; \beta_{n-1}|q_{n-1} > , \tag{5}$$

$$< q'_{n+1}|\beta_n \;=\; < q'_n|H \;-\; \alpha_n < q'_n| \;-\; \beta_{n-1} < q'_{n-1}| , \tag{6}$$

where $|q_0 > = \psi(0)$, $< q'_0| = \psi^*(0)$, $\alpha_n = < q'_n|H|q_n >$, $\beta_{-1} = 0$, and $\beta_n = < q'_n|H|q_{n+1} > = < q'_{n+1}|H|q_n >$. To compute $< q'_n|H$ in Eq. (6) one makes use of the relation $< q'_n|H = \{H^\dagger[< q'_n|]^\dagger\}^\dagger$, where $H^\dagger$ represents the Hermitian conjugate of the operator in Eq. (3), and the remaining $\dagger$ symbols signify the complex conjugate transpose of the indicated vector.

The matrix elements $< q'_n|H|q_{n'} >$ form an $N$-dimensional tri-diagonal complex symmetric representation of the operator $H$. The matrix, which we call $\mathbf{H}_N$, can be reduced to diagonal form by the operation $\widehat{\beta'} = \mathrm{diag}[\beta'_0,\ \beta'_1,\ \ldots,\ \beta'_{N-1}] = \mathbf{U}\mathbf{H}_N\mathbf{U}^{-1}$, where $\mathbf{U}\mathbf{U}^{-1} = \mathbf{1}$. Here $\mathbf{U} = [\mathbf{u}_0,\ \mathbf{u}_1,\ \ldots,\ \mathbf{u}_{n-1}]$, where the $\mathbf{u}_n$ are the eigenvectors of $\mathbf{H}$, and $\mathbf{U}^{-1}$ is the transpose (without conjugation) of $\mathbf{U}$. In this representation Eq (3) can be evaluated using the relation

$$\psi(z) = \mathbf{U}^{-1}\exp\left\{-iz\left[k - k(1 + \widehat{\beta'}/k^2)^{1/2}\right]\right\}\mathbf{U}\psi(0)\ . \tag{7}$$

Equation (7) generates accurate numerical solutions to the Helmholtz equation, including either loss or gain, and is extendible to arbitrary order.[4]

The development contained in Eqs. (1-7) is rigorously applicable only if the refractive index is invariant with $z$. One can, however, reasonably assume that the present formulation is applicable for adiabatic variation of refractive index with $z$. To test this assumption, we have calculated beam propagation in y-junctions formed from semi-conductor rib waveguides, involving large refractive index changes across the air-waveguide interface, i.e., of the order of $\Delta n = 2$. We have performed calculations for full y-angles from 8 to 90 degrees and have found both the Hermitian and nonHermitian methods to be fully robust in both cases. The required $\Delta z$ steps were of the order of 0.1 wavelengths, necessitated by wide radiation angles and the fact that it is not possible to define a meaningful reference k-vector for these problems.

## FINITE-DIFFERENCE TIME-DOMAIN

Interest has recently grown in applying microwave modeling techniques to optical circuit modeling[5-7]. One of the simplest, yet most powerful, microwave simulation techniques is the finite-difference time-domain algorithm (FDTD)[8]. In this technique, the differential form of the time-domain Maxwell's equations are discretized and all derivatives are approximated as centered differences. Minor algebraic manipulations on the resulting equations

produces a set of update equations that produce fields at a given time step from fields at the previous time step. The FDTD algorithm, then, is quite simple. Source fields are launched into the discrete grid and the FDTD equations advance these fields in time. At the boundaries of the grid, radiation conditions are applied that approximate a continuing, infinite space. We have also been using, and will discuss (using simulation video results) the FDTD in integrated optics design[9].

Because virtually no assumptions are made in the development of the FDTD method, the algorithm is able to represent a wide-range of physical effects. Waves can propagate in any direction, multiple reflections within structures can cause resonances, multiple modes of various polarizations can be launched, each of which may generate within the device an infinite spectrum of bound and radiation modes. The ability to model these types of general physical effects is what makes the FDTD method interesting to the field of optics. With this versatile technique we are able to predict the broadband behavior of geometrically complex optical interconnects.

To take full advantage of this power in three spatial dimensions and time requires a complete set of pre- and post-processing codes. The LLNL code suite TSAR consists of a set of graphical and computational tools arranged in a pipe-line, where information flows from tool to tool. At the beginning of the pipe, interactive grid generation tools accept the user's drawing of a problem and create the discrete finite-difference grid that represents the problem. At the end of the pipeline, advanced visualization tools transform field data from the simulation into animations, volume renderings, or whatever image is required to help the researcher interpret the data. Many problems of technological importance, however, require only two spatial dimensions and time for complete treatment. For these problems we have exploited the advantages of the reduced dimensionality and have compressed the code suite TSAR into a single graphical user interface called TSARLITE.

We have used this technique to study a number of integrated optical devices among which is a diffraction grating. We will show, among other things, how a transverse magnetic ($TM_0$) wave launched into a Bragg-grating loaded waveguide propagates through the diffraction structure and launches a directed radiated wave into the air. In previous, similar gratings, we have been able to send a radiation wave back in the direction of the incident wave. This problem, while geometrically simple, demonstrates a number of features of FDTD simulation that make it the technique of choice for many problems. First, the ability to handle coherent effects such as the Bragg reflections is essentially unique to FDTD because of its ability to handle propagation in *any* direction. This feature distinguishes FDTD from the commonly used *unidirectional* optical simulation methods. Second, FDTD can treat arbitrary polarization states and combinations thereof: a feature unique to FDTD. Indeed, most of the commonly used methods are limited to treating, at most, one polarization state at a time and, typically, are limited to the transverse electric field. The ability to accurately treat coherent effects, reflections, and wide spectral variations in material properties has made the study of grating-based devices and other complex structures a comparatively straightforward task. We find that the finite-difference time-domain method gives designers insights only revealed by complete vector EM fields.

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