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Design Tools for Photonics: Rising to the Challenge

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1. Introduction

Commercial success in the photonics marketplace dictates a full understanding of the product development lifecycle. Underpinning this success is the maximization of performance and minimization of product development time. These can be afforded at an early stage by employing computer design and simulation methodologies, enabling cost-effective and rapid evaluation of component performance prior to manufacture. This is particularly important in the development of photonics components, which tend to be largely dependent on processing and fabrication conditions.

Superior photonic circuit performance can be obtained by examining design alternatives, ideally by employing multi-dimensional optimization tools in design synthesis. The demands placed upon simulation software continue to increase dramatically as ever-more sophisticated processing techniques allow the development of complex three-dimensional structures, exploiting nano- and micro-scale materials and associated properties such as dispersion and non-linearity. Systems requirements demand that effects such as electromagnetic polarization, reflection, cross-talk and radiative profiles be modeled to a high degree of accuracy.

In the present discussion, we present a non-mathematical overview of the photonics modeling capabilities within the George Green Institute for Electromagnetics Research (GGIEMR) at Nottingham University, with examples on how state-of-the-art numerical simulation methods can be applied to satisfy the stringent requirements of component development. The research focus of the Institute is on electromagnetic analysis and simulation techniques, applied as a generic discipline across a variety of frequencies and applications. Many of the tools utilize common underlying themes, such as coupled-physics solutions, a requirement to deal with complexity, incorporation of diverse spatial and temporal scales, a necessity to adapt to new concepts and technologies in a concurrent manner, and importantly, the requirement for validation and comparison with experimental results.

2. Numerical Approaches

The Finite Difference Beam Propagation Method, FD-BPM [1] is widely accepted as the pre-eminent tool for photonic and electromagnetic modeling. The basis of the method is to replace the mathematical derivatives in the Helmholtz equation with corresponding finite difference expressions, whilst assuming that the field changes only slowly in an assumed propagation direction. The method simulates propagation in terms of this envelope, without the need to consider explicitly the rapidly varying aspects of the electromagnetic fields. Suitable boundary conditions, such as perfectly matched layers, are imposed at the edge of the computational window. A time domain version of the technique is also possible, where a time (rather than spatial) envelope is extracted.

One example that typifies the flexibility of the above approaches is the development of a laser model, produced by coupling an FD-BPM optical model self-consistently with an electrical-thermal equation solver [2]. The laser is an example of a ‘multi-physics’ problem (common in the field of computational electromagnetics), where diverse physical models, often with dissimilar timescales and lengths, are mathematically coupled in a systematic manner. Electromagnetic design tools must be capable of efficiently manipulating and extracting all relevant material properties in a readily useable form, from the fundamentally physical level to practical systems problems.

The FD-BPM considerably reduces the computational demand required by conventional time domain approaches, such as Transmission Line Modeling (TLM) [3] or Finite Difference Time Domain (FD- TD) [4], which sample at a fraction of the wavelength. The main disadvantage of the FD-BPM is associated with computational processing power. Demands on computer memory and processing times can increase dramatically with the size of the numerical problem. The three-dimensional case, in particular, will determine the computational viability of any particular formulation.

The bottleneck for many BPM algorithms is the requirement to solve a very large matrix problem for each elemental propagation step. Iterative solvers, coupled with significant algebraic pre-conditioning or ‘alternating direction implicit’ (ADI) schemes, are typically employed for three-dimensional schemes. Explicit BPM algorithms are attractive since each discrete propagation step only requires multiplication by a sparse matrix, and the algorithms exhibit very efficient parallelism. Most two and three level explicit BPM schemes are either unstable or require extremely small step sizes to ensure mathematical stability, although work by ourselves, and others, indicates that the Du Fort Frankel (DFF) variant allows stability in combination with relatively realistic step sizes [5].

The discrete parameterization of step sizes, referred to herein as ‘discretisation’, can also significantly affect the computational efficiency of any simulation. Staircase errors are a common problem for finite difference schemes implemented in uniform coordinate systems, causing an excessive mesh density to be required. We have avoided this by developing structure-related coordinate schemes for frequency domain techniques, in which the discretisation is made with respect to a parametric description of the geometry [6]. This methodology ensures that all material boundaries align with coordinate lines. Such schemes provide substantial computational advantages, for a given specification on accuracy, since the alignment of the propagation axis with geometry enables the use of paraxial ADI and DFF FD-BPM algorithms.

Other important advances include finite difference schemes that allow arbitrary positioning of dielectric boundaries within a mesh [7], a technique we have further refined to enable fine structures such as quantum wells to be accurately modeled using a relatively large discretisation. Embedding fine features within a coarser numerical grid is recurring theme across the whole range of our activities. These advances make it possible to undertake three-dimensional FD-BPM simulation of complex components such as the Arrayed Waveguide Grating (AWG), on a simple workstation, with sufficient accuracy to include the subtle phenomena that can influence performance in a system, such as attenuation, phase, cross-coupling, and radiation profiles.

The assumption of single-direction propagation is not acceptable for some situations. FD-BPM struggles with modeling, for example, facet reflectivities < -50dB, novel grating devices, wide angle scattering or coupling with evanescent fields. Reflective FD-BPM techniques are becoming more sophisticated for discrete reflections and for two-dimensional problems, although they remain to be completely investigated for three-dimensional problems and fully assessed with continuous reflections. This inherently iterative approach to interacting reflective discontinuities can be extremely slow to converge near resonances of a structure, but still remains a powerful tool. Figure 1, for example, shows the results from a three-dimensional FD-BPM simulation of the interface between an optical fiber and silicon-on-insulator (SOI) rib waveguide, where both components are mounted at an angle as well as incorporating an antireflection coating. The performance specification requires a fundamental power reflectivity below –40dB, when excited from the fiber, and insensitivity to vertical alignment errors.

Determining the modes of straight and curved waveguides remains an essential activity when designing photonic systems. Finite difference modal analysis techniques present the same advantages and disadvantages as the FD-BPM method, and despite the computational overheads, are still widely used. Other photonic components we have analysed include, but are not limited to, optical disk and micro-ring resonators.

Finally in this section we note that conventional time domain electromagnetic solvers such as TLM and FD-TD are extremely flexible and provide a rigorous numerical solution of Maxwell’s equations. The TLM method, originally developed by the Nottingham group, provides a common tool that can be applied, in principle, to a diverse range of materials and structures, including photonic bandgap crystals (which violate the inherent assumptions of the BPM), although computational resources usually limit the three-dimensional problems that can be addressed. A general TLM approach for the time-domain simulation of electromagnetic wave propagation in frequency-dependent non-linear materials has been reported [8]. We are exploiting this versatile technique in studies of the switching properties of non-linear gratings, extending earlier, more intuitive, implementation [9].

3. Semi-Analytical Approaches

Notwithstanding the discussions above, accurate simulation of a particular configuration does still allow certain approximations to be made. For example, the Free Space Radiation Mode (FSRM) method [10] can be used when transverse refractive index contrasts are less than 10% (with no restriction on the index contrast in the direction of propagation), and has proved invaluable in the analysis of buried waveguide structures such as semiconductor optical amplifiers. The Spectral Index (SI) method [11] and Half Space Radiation Mode (HSRM) method [12] can be applied to structures that employ a low-index (air) upper cladding. Within the remit of these physical approximations, semi-analytical analyses embrace general problems (including those involving loss, gain, radiation and reflections), and are extremely fast, accurate and robust design tools. We also include in this classification plane wave and localized function methods that we have used to study the modal properties of holey fibers.

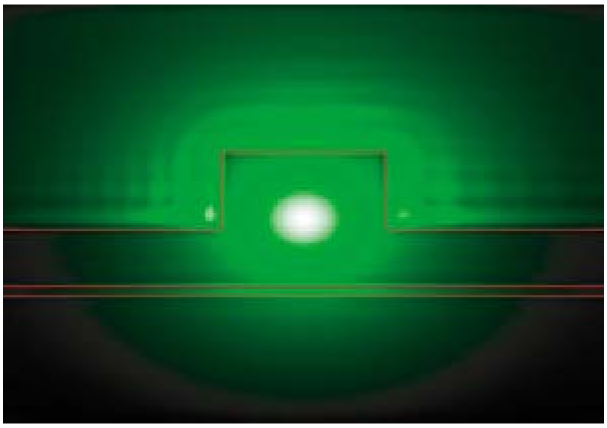

Figure 1: Scalar field excited by a single mode fiber (via angled facet) at the input of SOI waveguide.

An SI approach to simulating air-clad rib waveguide circuits has been described in [13]. The algorithm features truly piecewise linear models of rib geometries, solving a linear equation set that is very small compared to a numerical approach such as FD-BPM. This leads to an extremely fast and memory-efficient algorithm. Further advantage is gained since longitudinal discretisation lengths can be ten-times smaller than those required by FD-BPM (for comparable accuracy). The SI method has also been used [14] in a scattering matrix analysis of optical circuits utilizing rib waveguide geometries. In this situation, the optical circuit is divided into longitudinally invariant ‘blocks’ and a sufficiently complete leaky-mode spectrum is obtained for each block in a matter of seconds. The method employs mode polarization and accounts for both substrate radiation and slab mode leakage. Once the modal property of each block has been calculated, they are ‘joined’ using a scattering matrix, allowing a relatively simple representation of a more complex circuit.

Illustrative results for an electro-optic modulator, where the refractive indices of the parallel sets of waveguides are electronically modulated to control the optical output, are shown in Figure 2. The device has a maximum width of 18mm compared with a propagation length of nearly 3cm, yet the complete 3D simulation was undertaken in tens of minutes on a PC.

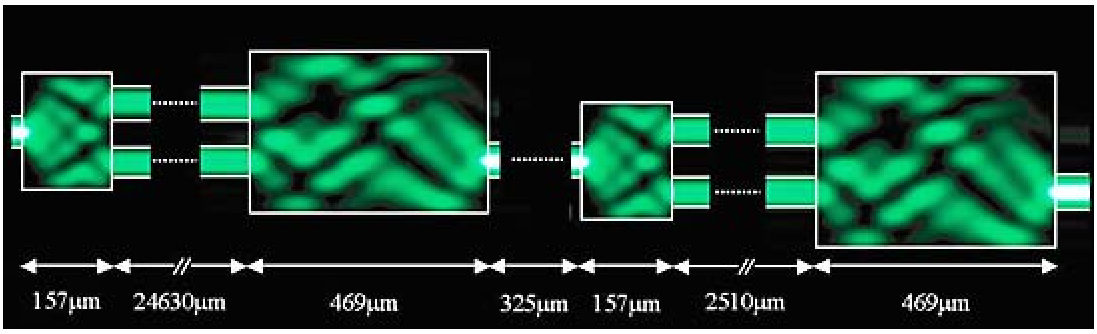

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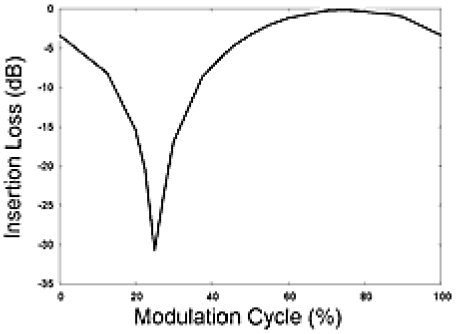
Figure 2: 3D Spectral Index simulation of an electooptic modulator (a_ optical field intensity within the device, operated at minimum insertion loss



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4. Hybrid Approaches

The complex fiber-to-chip coupling example discussed earlier (Figure 1) precludes a full, semi-analytical, analysis, whilst purely numerical methods demand considerable computational resources. In [15] we described a hybrid approach, with a single-mode fiber modeled using the FSRM method, coupled to an on-chip semiconductor rib waveguide, modeled using the FD-BPM. The two methods were linked using an iterative procedure and the associated theoretical results were in good agreement with experimental observations. The use of hybrid methods is another unifying theme in the research work of the GGIEMR.

5. Automatic Optimization

The use of optimization methods to automatically synthesize novel structures is beneficial to optoelectronic design. We have investigated how, by adaptively altering the accuracy of waveguide simulation during the optimization process, the synthesis of new designs can be sped up. Adaptive accuracy variation is achieved within two contexts: firstly, altering the required numerical tolerance within a single method, and secondly, by utilizing a hierarchy of differing methods. Having knowledge of the solution accuracy within optimization enables synthesis to user-defined accuracy. Combining optimization with, for example, adaptive semi-analytical simulations is a step towards the automatic CAD of optoelectronic components. We are presently extending these methods to run effectively on parallel processors.

6. Integral equation (analytical) methods

One approach, recently showed to have great promise for a wide class of problems, utilizes a combination of the Green's Function method and the Method of Analytical Regularization (MAR). Fast convergence and controlled accuracy of the algorithms emerge from a proper choice of the Green's functions, the use of high-order integration schemes, and an analytical treatment of singularities. We have successfully used such algorithms to simulate and design novel micro-laser and waveguide notch filter structures with improved characteristics [16].

We have simulated the tuning of whispering-gallery mode (WGM) filter frequencies and coupling efficiencies for micro-ring resonators, where refractive index and gain/loss variations are incorporated to correct for fabrication imperfections, and have designed-in intentional boundary imperfections to enhance Q-factors, reduce lasing thresholds, obtain directional light emission, and suppress parasitic modes (Figure 3a). We are applying the method to study surface roughness induced radiation loss and to estimate frequency shifts and loss-limited Q-factors in optical resonators, as well as exploring different micro-cavity shapes (Figure 3b) to design novel structures with improved filter characteristics (wider free spectral range, better tunability, enhanced coupling to straight waveguides, and lower sensitivity to fabrication tolerances).

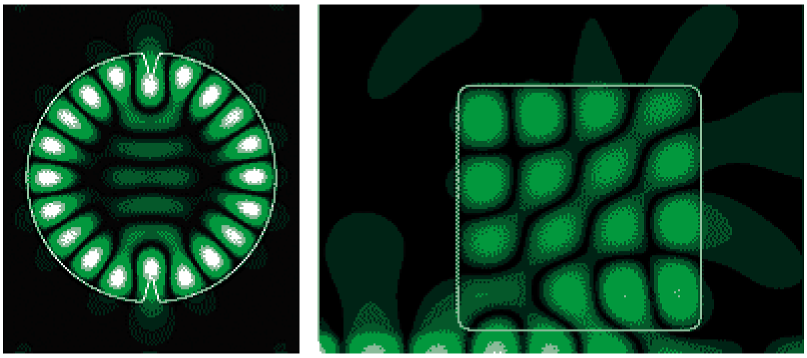

Figure 3: (a) notched microdisk laser operating on whispering-gallery modes. (b) square micro-resonator design.

We have combined the integral equation methods with the adaptive algorithms described in the previous section and used the resulting algorithm for a single-mode filter design which enables the suppression of parasitic resonances, optimizing for high-Q filtering at a given wavelength [17]. Further work is aimed at optimization of a micro-disk Vernier filter to selectively suppress WGM resonances and obtain a wider FSR compared with single-cavity filters.

We have also developed time domain integral equation techniques, discretised on an FD-like mesh [18]. These require, only, explicit discretisation in regions that differ from the assumed background medium and so, for many problems, offer a reduction in the algebraic problem size. Although the spatial meshing involves fewer samples, a time history is required at each point. Although this does tend to offset any advantage, it is possible that the saving in sampling within the three-dimensional space domain will outweigh the need to store samples in the one-dimensional time domain. Hybrid tools, combining numerical and integral equation approaches, certainly appear to be a fruitful way forward.

7. Conclusions

Many present day simulation and design tools for optoelectronics involve approximations and are ultimately limited by current computational hardware. We have endeavored to convey that a broad range of photonic devices and optical integrated circuits can be studied using a wide variety of numerical modeling methodologies, many of these being developed at our Institute, and exploited in automated design optimization. The next generation of simulation software must aim to eliminate such limitations, ideally solving the vector Helmholtz equation subject to open boundary conditions. Advances in our understanding of integrated design methodologies, and novel approaches, combined with advances in available computing power, will ultimately enable rapid simulation and facilitate rapid prototyping of photonic components and circuits for commercial exploitation.

8. References

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