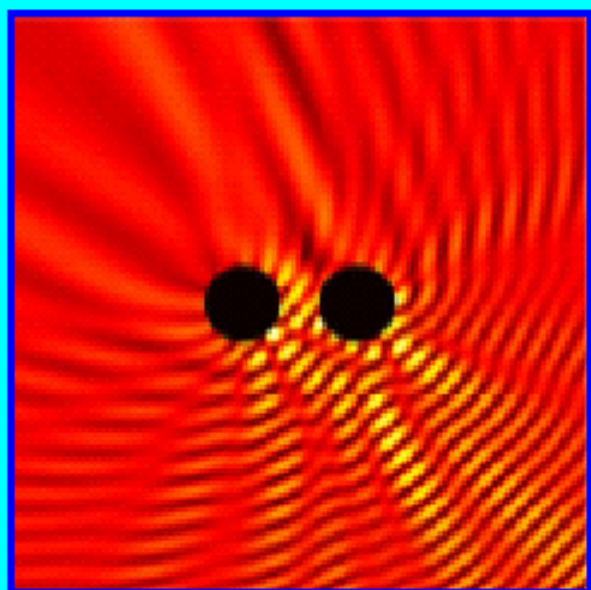


Institute *of* Physics

# Newsletter

*of*

The Computational Physics Group



Fall 2004

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Picture of scattering from two cylinders courtesy of E. J. Grace and M. W. McCall.

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## **Foreword**

*David C. Hutchings, University of Glasgow*

The simulation and design of photonic materials, devices and systems is an active area of research and has had a major impact in the innovation and commercialisation of photonics in telecommunications, displays, remote sensing and many other sectors. The general increase in demand and capacity of computational resources has recently led to the designation and promotion of e-Science within the United Kingdom. However, computational photonics is one of the areas of e-Science which has already been making an impact over several decades.

In this newsletter, we provide an overview of the types of problems which computational photonics can solve. Most of the leading UK research groups have provided a snapshot of the type of research they are currently engaged in. If you find these topics of interest, you will be able to hear these groups present their research on a half-day meeting on *Computational Photonics* in Glasgow on Wednesday 2 February 2005 sponsored by the IoP Computational Physics Group and the IEEE Lasers and Electro-Optics Society Scottish Chapter. For more details please contact Prof. David Hutchings (D.Hutchings@elec.gla.ac.uk).

## **Overview of Electromagnetic Solvers for Photonics**

*David C. Hutchings and John M. Arnold, University of Glasgow*

The computer simulation of photonic devices and systems not only allows the conception and explanation of experiments, but also enables the design and rapid prototyping of commercial devices and systems. Historically, the limited computational power available required that the models for devices and materials were substantially simplified. Now, as the computational power available continues to be driven by Moore's Law, greater fidelity is possible by avoiding

these approximate models and instead running *ab initio* models in addition to being able to tackle a denser discretisation. More complexity can also be studied by combining the electromagnetic solver with fundamental descriptions of the microscopic and/or quantum processes in the media. For example, in the case of semiconductor lasers it is necessary to simulate the electromagnetic fields in the device, which involves the solution of Maxwell's equations in media with complex boundaries with sources formed by the distribution of electronic charges in the dielectric polarisation. These electrons are in turn described by quantum mechanics in a solid state medium, requiring a simulation of the bandstructure of the medium and the electron dynamics which results form the particular bandstructure. In order to represent the noise characteristics of a laser it is necessary to have models of the electromagnetic field that are quantised, and to consider the statistics of the coupling of electrons and photons in the electromagnetic field. Each of these separate models is a large scale mathematical construction which it is impossible to solve in analytical form for any realistic problem. Moreover, the systems are in any case all coupled together so that one of them cannot be solved without knowledge of the solutions of the others. Coupling of these models tends to be highly nonlinear and often requires the dynamics on ultrashort timescales. Because of the complexity of the models, and the nonlinear coupling among them, a large body of approximate theory has grown up in order to reduce the tasks of computing the dynamics of realistic laser devices. In fact the current state of knowledge of laser physics is an enormous aggregation of such approximations.

In the present article we provide an overview some of the more common methods for electromagnetic solvers used in photonics. The largest class of devices and interconnects that have been simulated by the techniques described here are waveguides [1], but free-space propagation, cavities and photonic microstructures also make substantial use of these methods.

The starting point in electromagnetics is Maxwell's equations

$$\nabla \cdot \mathbf{D} = \rho \tag{1}$$

$$\nabla \cdot \mathbf{B} = 0 \tag{2}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t} \tag{3}$$

$$\nabla \times \mathbf{H} = \mathbf{j} + \frac{\partial \mathbf{D}}{\partial t} \tag{4}$$

where the constitutive relations are

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} = \epsilon_0 \epsilon_r \mathbf{E} \quad (5)$$

$$\mathbf{B} = \mu_0 (\mathbf{H} + \mathbf{M}) = \mu_0 \mu_r \mathbf{H} \quad (6)$$

$$\mathbf{j} = \sigma \mathbf{E} \quad (7)$$

The Finite Difference Time Domain (FDTD) method [2–6] is a direct solution of Maxwell's equations obtained by replacing the space and time derivatives with finite differences. It is normal to use a leap-frog technique where the space and time derivatives for the electric and magnetic fields are central-difference in nature and second order accurate with error  $\mathcal{O}(h^2)$ . In three spatial dimensions this usually takes the form of the Yee cell construct.

Now the FDTD method is well established in RF modelling but has only just started to be used for photonic applications in the last decade or so. [7, 8] To see the limitations consider the simulation of a typical single-moded waveguide of  $\sim 1$  mm length at optical communications wavelengths. Taking a relatively coarse step-size of  $\lambda/10$  in the material requires a spatial discretisation of the order of  $100 \times 100 \times 10000$  or approaching a GigaByte of storage per field quantity (assuming double precision). In addition, to simulate  $\sim 1$  ns will require the order of  $10^{16}$  floating-point operations. Therefore current FDTD simulations in photonics tend either to restrict the number of spatial dimensions to 1 or 2, and/or to analyse devices with a strong optical confinement in all spatial dimensions, such as Vertical Cavity Surface Emitting Lasers (VCSELs) or Photonic Microstructures. Currently, in addition to the substantial number of in-house codes produced by universities and other research institutions, there are a number of commercial FDTD implementations available from RF and photonics simulation companies.

Taking the usual assumptions of no free charges and nonmagnetic media, Maxwell's equations can be combined to give the Helmholtz wave equation.

$$\nabla^2 \mathbf{E} + \nabla (\epsilon^{-1} \mathbf{E} \cdot \nabla \epsilon_r) - \mu_0 \sigma \frac{\partial \mathbf{E}}{\partial t} - \frac{\epsilon_r}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0 \quad (8)$$

Now to facilitate a substantial increase in step-size the following approximations are usually employed. First it is assumed that wave propagation is in one direction only. For example, a monochromatic wave propagating parallel

to  $+z$  can be represented.

$$\mathbf{E}(x, y, z, t) \rightarrow \frac{1}{2} \left( \tilde{\mathbf{E}}(x, y, z) e^{i(kz - \omega_0 t)} + \tilde{\mathbf{E}}^*(x, y, z) e^{-i(kz - \omega_0 t)} \right) \quad (9)$$

Note that this method therefore cannot be directly applied to two-way propagation such as gratings or cavities. Second, the Slowly Varying Envelope Approximation (SVEA) allows the second-order derivative of the envelope in  $z$  to be neglected.

$$\frac{\partial^2 \tilde{\mathbf{E}}}{\partial z^2} \ll \frac{\partial^2 \tilde{\mathbf{E}}}{\partial x^2}, \quad \frac{\partial^2 \tilde{\mathbf{E}}}{\partial y^2}, \quad \frac{n_0 \omega}{c} \frac{\partial \tilde{\mathbf{E}}}{\partial z} \quad (10)$$

The resulting parabolic partial differential equation is known as the paraxial wave equation as it is valid for wave propagation limited to small angles with respect to the  $z$ -axis.  $\nabla_{\perp}$  is the vector differential operator in the transverse dimensions  $(x, y)$  only.

$$\frac{2in_0\omega_0}{c} \frac{\partial \tilde{\mathbf{E}}}{\partial z} = -\nabla_{\perp}^2 \tilde{\mathbf{E}} - \nabla_{\perp} \cdot (\boldsymbol{\varepsilon}^{-1} \mathbf{E} \cdot \nabla_{\perp} \boldsymbol{\varepsilon}_r) + (n_0^2 - n^2(x, y, z)) \frac{\omega_0^2}{c^2} \tilde{\mathbf{E}} - i\omega_0 \mu_0 \sigma \tilde{\mathbf{E}} \quad (11)$$

Here we have substituted  $k = n_0 \omega_0 / c$  and  $n_0$  is the reference refractive index.

The Beam Propagation Method (BPM) is the means of solving eqn. (11) to obtain the transverse field profile as a function of the propagation direction  $z$  given an initial transverse field profile at  $z = z_0$ . [9–11] This is the analogy of the physical situation of coupling a beam of light into a waveguide and observing its subsequent propagation. In order to accommodate abrupt interfaces between different media we refer back to Maxwell's equations and use the corresponding boundary conditions which specify continuity of normal components of  $\mathbf{D}$  and  $\mathbf{B}$ , and continuity of transverse components of  $\mathbf{E}$  and  $\mathbf{H}$ . Parabolic partial differential equations have many examples, such as the heat equation, and there are a multitude of available techniques. Some of the common techniques applied to the BPM include finite difference, finite element and Fourier (for rectangular geometry) or Hankel (for cylindrical geometry) transforms. There are also various approximations which can reduce the complexity of the simulation; one of the most common is the Effective Index Method [12] which reduces a three-dimensional problem to a two-dimensional one. Again, there are many BPM implementations used in research plus a number of companies which offer a BPM as part of their photonics simulation packages.

Mode-solvers provide the steady-state solutions  $\mathbf{e}_i(x, y)$  to eqn. (11) by setting  $\partial\mathbf{E}/\partial z = 0$ . This is a boundary value (usually setting zero field distant from the structure for guided modes) problem with an eigenvalue given by the effective refractive index  $n_0$ . In contrast, the previously discussed cases fall into the category of initial value problems. Again there are a number of numerical techniques appropriate to this type of solution including finite difference, finite element and shooting method. [13, 14]

For a given device geometry, the set of modes, including the continuum of radiation modes in addition to the discrete bound modes, form a complete set. Therefore any field distribution can be represented as a summation over these mode profiles.

$$\tilde{\mathbf{E}}(x, y, z) \rightarrow \sum_i \mathbf{e}_i(x, y) u_i(z) \quad (12)$$

Now perturbation theory allows the approximation of this infinite sum as a finite sum over the most relevant modes for structures which are a sufficiently close relative of the original, usually simpler, structure for which we have obtained the set of modes. This mode expansion technique allows for a relatively simpler analysis of some photonics problems in comparison to the FDTD or BPM techniques, particularly where the structure varies along the propagation direction. Some examples are weak gratings, where the set of modes cover both forward and backward propagation directions, tapered waveguides, coupled waveguides, such as directional couplers and waveguide arrays.

In a similar vein to modal expansion techniques, there are some problems which can be analysed by expanding the field profile as a summation of plane waves (modes of free space). Computing the propagation of monochromatic plane waves is normally straightforward. The device structure can be incorporated by applying the usual boundary conditions for electric and magnetic fields at interfaces. These relations can be expressed as a matrix equation giving rise to the transfer matrix method. This was applied to the simulation of thin film optical filters half a century ago [15], but has also been applied more recently to photonic microstructures [16, 17].

So far we have assumed that the medium's response through the polarisation  $\mathbf{P}$  is (1) instantaneous and time-invariant and (2) linear, i.e.  $\mathbf{P} \propto \mathbf{E}$ . There are many interesting examples where computational photonics techniques are being currently extended to devices and systems which do not meet these criteria. Incorporating a non-instantaneous polarisation, or equivalently a frequency

varying or dispersive dielectric constant, is nontrivial in the case of time domain techniques. Note that eqn. (5) is a multiplication in the frequency domain which corresponds to a convolution in the time domain. Therefore, in principle, the field values are required at all earlier times, severely increasing the storage and computational requirements. As a consequence FDTD solvers tend to be restricted to the special cases of Debye or Lorentz dispersion where the envelope of the dielectric constant in the time domain is a decaying exponential. This allows an incremental determination of the convolution integral reducing the storage requirements to a single or few additional quantities.

The most complete methods for incorporating the polarisation evolution is by adding auxiliary differential equations describing the microscopic state of the medium. [18] This could be a case of rate equations for carrier or heat diffusion, or could include quantum effects, for example by incorporating Bloch equations [19–21] or Semiconductor Bloch equations [22, 23] in which the density matrix is evaluated at the same set of nodes as used for the electromagnetic fields in the FDTD or BPM techniques.

Common methods of including nonlinear and dispersive effects are through series expansions. Nonlinear effects can be incorporated by a power series expansion in the electric field.

$$P = \epsilon_0 \left( \chi^{(1)}E + \chi^{(2)}E^2 + \chi^{(3)}E^3 + \dots \right) \quad (13)$$

Strictly speaking, eqn. (13) should be in vector form with the  $n$ th order susceptibility  $\chi^{(n)}$  given by a rank  $n + 1$  tensor. Additionally, the sum or difference of the electric field frequencies should be taken. Hence for a monochromatic input, the second-order polarisation term is limited to double the frequency  $2\omega_0$  (second harmonic generation) or zero frequency (optical rectification). The third-order term can give rise to a polarisation component at the original frequency  $\omega_0 = \omega_0 - \omega_0 + \omega_0$ . This manifests itself as nonlinear refraction (optical Kerr effect) or nonlinear absorption.

The series expansion of the dielectric constant (or refractive index) is normally done by using a Taylor expansion around the carrier frequency  $\omega_0$ .

$$\epsilon_r(\omega) = \epsilon_r|_{\omega_0} + (\omega - \omega_0) \left. \frac{d\epsilon_r}{d\omega} \right|_{\omega_0} + \frac{1}{2}(\omega - \omega_0)^2 \left. \frac{d^2\epsilon_r}{d\omega^2} \right|_{\omega_0} + \dots \quad (14)$$

A non-zero first order term provides for a group velocity being unequal to the

phase velocity, but otherwise does not provide a changing waveform. A non-zero second-order (and higher order) term results in group velocity dispersion (GVD) that generally results in pulse chirping and broadening. Analysis of this type of system normally defines the envelope  $\tilde{\mathbf{E}}$  to have a slowly-varying time dependence, which results in a term in the evolution equation containing the second-order time derivative  $\partial^2 \tilde{\mathbf{E}} / \partial t^2$ . The combination of GVD and self-phase-modulation (nonlinear refraction) gives rise to the Nonlinear Schrödinger Equation [24]

$$i \frac{\partial u}{\partial z} = \frac{1}{2} \beta_2 \frac{\partial^2 u}{\partial t^2} - \gamma |u|^2 u \quad (15)$$

where  $\beta_2 \propto d^2 \epsilon_r / d\omega^2|_{\omega_0}$  specifies the group velocity dispersion and  $\gamma \propto \chi^{(3)}$  specifies the optical Kerr effect. This equation supports soliton solutions in the case of anomalous dispersion and self-focussing nonlinearity. Interestingly the same form of equation is obtained to describe spatial solitons where the second-order spatial derivative describing diffraction (see (11)) replaces the time derivative.

In summary, computational photonics has a history spanning several decades. However in order to make problems tractable with the contemporary computational resources the problems to be tackled required simplification and application of approximations. This article indicates some of the common approximations applied to electromagnetic solvers in photonics. One of the costs in this approach is the lack of flexibility in that a particular set of approximations may only be appropriate for a limited family of structures. The topic is now at a stage where the Moore's Law exponential rise in computational power is allowing more fundamental generic techniques, such as FDTD, to become increasingly popular. In addition more complex models are being investigated incorporating quantum, microscopic and macroscopic processes in the materials, devices and systems.

In this newsletter a number of summaries are presented illustrating the current range of research in computational photonics and the development of models and methods to be able to simulate increasingly complex devices and systems.

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## **Microscopic Modelling of Semiconductor Optoelectronic Devices**

*Ian Galbraith, Heriot-Watt University*

Semiconductor optoelectronic devices such as semiconductor lasers and amplifiers play a key role in many of today's technologies - optical data communication, DVD players, laser printing and materials processing. The optimization of these devices is essential to providing the functionality and stability required of real world applications e.g. high power output, wavelength stability or low threshold current.

The heart of such devices is the active region where electrons and holes, which have been electrically injected into the device, undergo stimulated emission producing a coherent photon. The details of this seemingly simple process are affected by many interactions both internal and external. The electrons and holes scatter amongst themselves via their mutual Coulomb interaction. They also exchange energy and momentum with the lattice via phonon scatterings thereby cooling or heating the carrier plasma. These scatterings take place between the allowed energy states in the conduction band (for electrons) and the valence-band (for holes). In practice these states do not have a simple text-book parabolic energy dispersion with a fixed effective mass but have a complex web of allowed states. There is also the optical wave propagation to consider, as the carriers affect not only the gain/absorption of the light but also the refractive index and hence phase of the beam.

Given this complexity it is perhaps not surprising that empirical rate equation models, although appealing in their simplicity, cannot really describe the underlying physics in sufficient detail to adequately be used for quantitative modelling. For this we need a microscopic model in which the physics is computed correctly. The starting point for this is the Hamiltonian which describes the electrons and holes and their interactions with each other, with the lattice and with the light field. This is used to generate a set of equations of motion of relevant physical quantities. To lowest order in the interactions these are the electron and hole populations (in each allowed state) as well as the optical polarization generated by the light field. Usually the underlying bandstructure for the semiconductor is computed separately by *ab-initio* or *k.p* models and is

taken as input to these kinds of calculations - but its influence is key to having an accurate model.

Typically there would be of order of a thousand or so first order differential equations that need to be solved. The numerical difficulties arise in treating the singularities in the Coulomb interaction (both in real space and in k-space). The solutions to these microscopic equations then provide the polarization source term to the propagation equation for the light field. If there is no spatial symmetry around the light propagation direction the number of equations to be solved is essentially squared and the problem becomes more cumbersome but tractable with today's machines. Differential equations for higher order correlations such as excitonic effects can also be obtained by the same procedure but in this case the evaluation of the right hand side of these equations becomes very demanding as multi-dimensional integrations have to be done at each time step. Parallel implementations are so far hampered by the high degree of coupling between the equations. For practical simulations this remains a challenge for a future generation of hardware.

In summary microscopic simulations for semiconductor optoelectronic devices can provide quantitative information about device performance and commercial offerings based on these approaches are already on the market.

## **Computational Photonics in Salford**

The photonics and nonlinear group in the University of Salford, Joule Physics Laboratory, led by Professor A. D. Boardman has been enthusiastically working towards the production of software to study many aspects of photonics science. Starting from scratch the group has developed theoretical methods and advanced numerical techniques to analyse complex waveguides. The latter can be filled with nonlinear materials, magneto-optic materials, or negative index media. The Group is now specialising in left-handed metamaterials and they deploy a powerful finite-element solver, which was entirely developed in the laboratory. This software has a novel mesh-generator module embedded in a state-of-the-art program. To pursue the study of complex

waveguides it is necessary to develop software based around artificial intelligence. This is needed to estimate the TM/TE conversion efficiency in the kind of asymmetric waveguides needed for optical isolators in the chip-level control of lasers that lies at the heart of our Cambridge/Glasgow collaboration in this area. Specifically we use Genetic Algorithms that are in essence a natural selection process, deployed to compute through the agency of an optimum solution. It seems that Genetic Algorithms can be used as method to achieve performance optimization in a wide range of disciplines, but it is the rapidly growing area of photonics, and especially biophotonics, that they come into their own. This kind of software is a pivotal addition to any experimental platform in the design of the most appropriate configuration when design tolerances play an important role.

The simulation of new materials, such as the left-handed materials (an important class of metamaterials) is proceeding at a fast pace through the implementation of finite-difference time-domain (FDTD) software. Yet again this software has been entirely produced in the laboratory, FDTD is very powerful because it can introduce rather general constitutive relationships directly into Maxwell's equations without any further approximation. Real problems can then be addressed in a way that is suitable for the description of highly dispersive materials. A variety of problems have been investigated in Salford using this technique. They include negative refraction that appear to bend light "the wrong way" upon refraction, spatial solitons at interfaces optical vortex phenomena, dissipative solitons and a collaboration with Cambridge and Southampton that hinges upon a fascinating study of supertoroidal interactions that will be important in drug design. The Group emphasis now is upon parallel coding and upon developing more techniques to indulge study our main passion for nonlinear optics.

## **Photonics Modelling Research at City University London**

Following the development of semiconductor lasers and low-loss optical fibres in 1960s, the progress of optical technology has been most significant

in the field of optical communications. Today, the world is connected with millions of kilometres of silica fibre forming the global information technology highway. As optical technology has reached maturity during the last two decades, the associated devices have themselves become more complex. The optimization of such advanced devices requires an accurate knowledge of their lightwave propagation characteristics and their dependence on system fabrication parameters. Unfortunately, analytical techniques are not adequate to model lightwave devices without significant approximations. Therefore, the optimization of existing, realistic designs or the evaluation of new designs for optoelectronic devices and sub-systems has created significant interest in the development and use of effective numerical methods.

The Photonics Modelling Group at City University has been working for more than two decades on the development of rigorous modelling techniques for integrated optic and fibre optic components and sub-systems. This involves the computer-aided characterization of linear, nonlinear, anisotropic and active optical-guided-wave devices. The main expertise of the Group has in the development of powerful, versatile, full vectorial, accurate and numerically efficient finite element method (FEM)-based design tools to investigate the characteristics of photonic devices and optoelectronic systems. Research projects on high-speed optical modulators, spot-size converters, polarization rotators, WDM components, compact bend designs, VCSELs, photonic crystal fibres and Bragg gratings have been supported, amongst others by EPSRC, the EU, the Royal Society, the British Council, QinetiQ, Nortel, Agilent, Marconi, Bookham, and Corning.

Optical waveguides not only connect all the optical components inside optical systems, but also are the basic building blocks of many photonic devices. The full vectorial H-field based finite element method (VFEM) has been used to characterize accurately lightwave propagation through a wide range of waveguides, such as semiconductor ridge and titanium diffused LiNbO<sub>3</sub> waveguides. This method is particularly advantageous because of its applicability to waveguides with arbitrary shapes and arbitrary refractive index profiles. The finite element formulation, using the accurate vector H-field formulation which is "exact-in-the-limit", is also valid for anisotropic materials.

However, when guided-wave structures have a finite number of junctions, it is necessary to find their transmission and reflection coefficients at the discontinuity junction and a rigorous and full vectorial numerical approach has been

developed by using the least squares boundary residual program. To deal with a more general three-dimensional axially nonuniform guided-wave structures, a full vectorial beam propagation method (BPM) has been developed to study the evolution of the optical field along such an optical guided-wave devices or sub-systems. The BPM code developed at City University is based on the FEM, which uses arbitrarily nonuniform discretisation in the transverse plane and is computationally more efficient than the commercially available finite difference method-based BPM.

It is generally known that optical modes in semiconductor waveguide are hybrid in nature. For a perfectly uniform optical waveguide with low index contrast, modal hybridness may not be a major issue. However, practical waveguides with non-vertical side walls, with bends, with thermal stress or applied pressure, with nonuniformity along the axial direction, both polarization dependent loss and polarization conversion are major concerns for optoelectronic systems. Circularly symmetric optical fibre cannot maintain the polarization states of the optical signals, whereas the performance of many photonic integrated circuits (PICs) critically depends on the incoming polarization states. So, in the design of polarization diversity optical communication systems, polarization splitters, polarization rotators, and polarization controllers are the key components to control and manipulate the polarization state of the signal. Various design concepts for the designs of polarization splitters, polarization rotators, polarization controllers have been undertaken, with some such projects being directly funded by industries, and patent applications are being evaluated.

Many directional couplers, Mach-Zehnder and MMI-based devices, such as power splitters, combiners, narrow-band filters, high-speed modulators have been developed. In the design of high-speed modulators, it is necessary to match the microwave and optical wave velocities and also reduce both conductor and dielectric losses. The FEM-based microwave model has been developed to optimise electrode design to increase the bandwidth of such modulators. Currently, several industrial groups are developing 40 Gbs modulators and with the collaboration from industry, both deep-etched GaAs, shallow-etched InP-based electro-optic modulator designs have been considered. Similarly titanium diffused and annealed proton exchanged LiNbO<sub>3</sub> modulators, with both unetched and etched designs have been considered.

Most of the advanced active photonic devices available produce non-circular

spot-sizes, 1 to 3 microns in dimensions. On the other hand, standard single mode telecommunication fibres produce circular but much larger spot-sizes, about 10 microns in diameters. One of the major problems arises during the coupling of a photonic device to an optical fibre is that more than 80% of the power can be lost due to their rather different spot-sizes. Recently, various laboratories have been considering the use of monolithically integrated spot-size converters to slowly expand the spot-size of an active photonic device and improve the coupling to an optical fibre. Both the FEM-based modal solution and the FEM-based BPM have been used to study the evolution of spot-size for various adiabatically tapered spot-size converters to achieve maximum coupling efficiency.

Photonic crystal fibres, a recent development with real significance for sensing and communications, are showing great potential with adjustable spot-size and group velocity dispersion. The FEM and FEM-BPM approaches have been used to study single mode operation, spot-size, hybridness, material nonlinearity, leakage loss, group velocity dispersion, modal birefringence, and the effects of stress on modal degeneration have been studied.

## **Modelling Monolithic Mode-locked Semiconductor Lasers**

*E.A. Avrutin, University of York*

Mode locking (ML) is usually described as the regime of laser generation whereby the laser emits light in several longitudinal modes with precisely equidistant frequencies and roughly equal phases. In such a regime, the laser emits a train of ultrashort (shorter than the round-trip) optical pulses with a repetition frequency  $F$  near the cavity round-trip frequency or its harmonic. ML is usually achieved either by modulation of the laser net gain at a frequency  $F$  or its (sub)harmonic (active ML) or by exploiting nonlinear properties of the medium, usually by introducing a saturable absorber (SA) into the laser cavity (passive ML). The combination of these methods is known as hybrid ML.

ML in monolithic semiconductor laser diodes is attracting considerable interest[1], firstly, for an increasing number of practical applications and, secondly, from the scientific point of view, as an important prototype system in nonlinear dynamics and as a manifestation of high-speed nonlinearities in active semiconductor media. Theoretical models, ideally with predictive capabilities, are therefore useful for detailed understanding of the physics of these devices, analysis of their behaviour and, ultimately, optimisation of laser design and operation regimes.

Modelling ML lasers can benefit significantly from the progress in the modelling of semiconductor lasers in general. However, there are several significant specific features of ML lasers that are to be borne in mind :

- The design of a ML laser is by definition relatively complex, with at least 2 separately biased sections, one of which is the forward biased gain section whilst the other, the modulator section for active ML or the SA for passive ML, is reverse biased. Depending on application, other elements may need to be included as well. On the other hand, ML essentially involves longitudinal phenomena, so it is often enough to use models operating in 1D+T, unlike say, VCSEL modelling.
- Dynamics of ML semiconductor lasers can be rather rich and include, generally speaking, several very different characteristic time scales: from the pulse scale (sub-ps to a few ps) to the slow transient scale (the so-called supermode competition, typically 1-100 ns). Moreover, ML lasers are known to be prone to dynamic instabilities of various kinds, from periodic self-pulsing envelope to chaos, particularly under modulation for hybrid ML
- The device behaviour may be sensitive to a large number of parameters, some of which are not very well known. Relatively modest changes in parameters (e.g. current, or saturable absorber recovery time in hybrid or passive mode-locking) can change the device behaviour qualitatively, moving it from one operation regime to another
- Comparison with experiments, which is the ultimate test for any model, is not always straightforward; for example, some instabilities may be difficult to register experimentally and may just show as increased noise.

The peculiarities of semiconductor lasers as opposed to different active media mean that the traditional analytical theory of mode-locking developed in the 1970s has some important limitations for semiconductor lasers. New models have therefore been developed lately. The model that has currently become the approach of choice in most in-house and commercial laser simulators is the Travelling-Wave Time-Domain model. The approach is very versatile, accurate, and powerful and covers most fast laser constructions, including ML lasers - however, special care is needed for some aspects of ML, notably fast nonlinearities. A more specialised model is the mixed time-frequency domain Dynamic Modal Analysis[2], which is less generic but can be very efficient and has the logical advantage of describing steady-state ML as a stationary solution. The combination of the two approaches can be expected to cover all the laser designs and regimes of interest.

With the set of dynamic phenomenological models established, the next step towards achieving true predictive capability is to integrate these models with first-principles calculations of the semiconductor properties. In most cases, the modeling of the gain media can benefit from the advances in modeling "ordinary" semiconductor lasers; however, there are some cases when specialist analysis is necessary. One case is the temporal response of the reverse-biased quantum well SAs, where it is necessary to take care of the processes of carrier removal from the reverse biased structure, carrier-induced electric field screening, as well as the absorption dependence on the electric field and carrier density. Our recently developed Delay-Differential model is an efficient approach suitable for integration with time domain laser simulators[3].

The second case is the analysis of the ML potential of quantum dot (QD) lasers. In this case, the discrete energy spectrum of the active material and the associated strong spectral hole burning need to be taken into account. Our recent studies[4] combine the rate equations for the populations of quantum dots with the dynamic modal analysis of the laser radiation to predict the possibility, with an advanced laser design, of turning the broad spectrum of QD lasers into sub-ps ML pulses.

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## Calculation of Losses in 2D Photonic Crystal Membrane Waveguides Using the 3D FDTD Method

*M.J.Cryan, D.C.L.Wong, I.J.Craddock, S.Yu, J.Rorison and C.J.Railton, University of Bristol*

There is much interest in 2D photonic crystal waveguides (2D PhC-WGs) which show the potential for low-loss guiding [1] and enhanced functionality over simple, uniform, high contrast waveguides due their strong confinement and dispersion properties [2]. The most promising results for 2D PhC-WGs are being found in structures with strong vertical confinement. These are known as a membrane guides and can be either suspended in air or used in a Silicon-Insulator (SOI) configuration [2]. This high vertical contrast leads to wide wavelength ranges where the propagating modes are below the air light-line which implies zero coupling to radiation modes and hence zero loss, neglecting effects such as surface roughness and material loss. Whilst measured loss values in PhC-WGs are reducing quite rapidly, there is still a strong requirement to fully understand the lower limits that can be achieved in the various guiding technologies. Below the light-line the limiting factors will be surface roughness and material loss which is well understood for standard high contrast waveguide [2]. However, in the more complex propagation regimes possible in PhC-WGs further work is still required. Above the light-line is a more interesting case where intuitively one would expect high losses, however, regions of low loss guiding have been predicted.

Here we will use a 3D FDTD code which has been developed over seventeen years to study losses in these air membrane guides. Figure 1 shows the details of structure to be investigated. This is being used a benchmark structure as part of a COST P11 modelling exercise [3] and these results will appear in [4]. The method used is being called the FDTD Cut-Back method since it is very similar to the approach used when physically measuring the losses in these and many

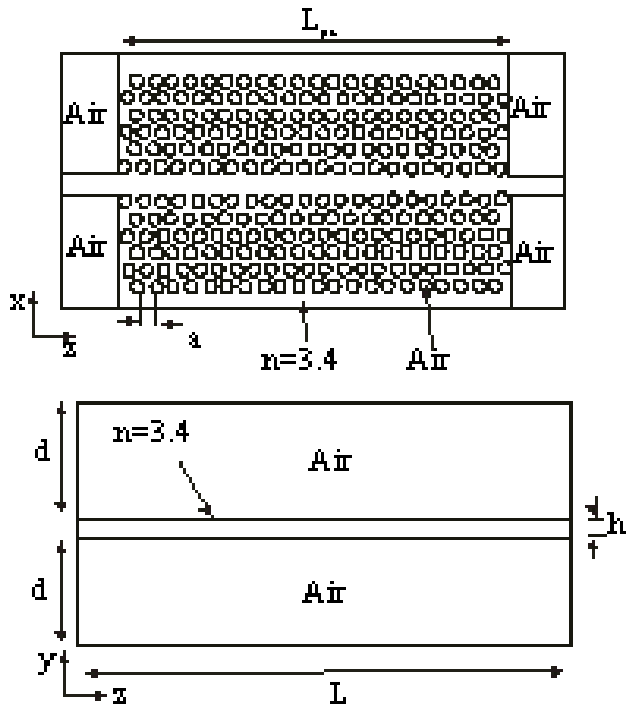


Figure 1: Photonic Crystal membrane waveguide with  $r/a=0.3016$ ,  $a=430.55\text{nm}$ ,  $h=0.6a=258.3\text{nm}$ ,  $L_{1,2,3}=6.028\text{m}$ ,  $10.76\text{m}$ ,  $19.37\text{m}$ ,  $L_{pc1,2,3}=11a$ ,  $22a$ ,  $42a$ ,  $d=870\text{nm}$ , W1 guide in  $-K$  direction,  $n=3.4$

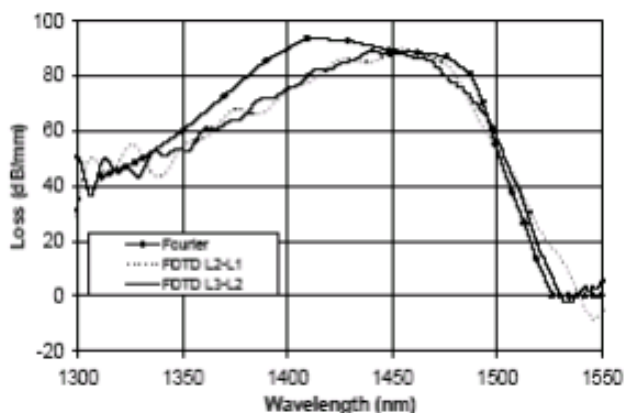


Figure 2: Comparison between loss results for Fourier method and 3D FDTD

other types of waveguides. The approach is to model the transmission through two different length waveguides. The difference between these two results, divided by the length of the waveguide gives the loss in dB/mm. The larger the difference in the two lengths the more accurate the results will become – this is a challenge for both measurement and modelling, as can be seen the longest modelled device is around 20m long, in reality devices with lengths of millimetres have now been fabricated. This would take a very big computer to model – though Bristol does have a 260 machine Pentium 4 cluster that we are working on implementing parallel FDTD which could easily handle millimetre long devices. The down side to FDTD modelling is the length of time taken for the simulations to run, using a single Pentium 4 machine the longest simulation here takes 140 hours. Whilst this may seem very long – at the end of this run FFTs are performed which give frequency domain information across a very wide bandwidth, and thus it is very competitive with other faster frequency domain methods in terms of time/frequency point.

The key feature to get accurate results is the use of modal excitation. This is an approach developed at Bristol which first solves for the fundamental mode of the input photonic wire waveguide, in the 2D cross section. This mode is then

launched into the 3D simulation. This excites the waveguide in a very realistic way. This then allows us to define Modal Scattering parameters, so we look at the power transmitted through the waveguide and back into fundamental mode of the output guide. This approach coupled with Perfectly Matched layer boundaries to absorb all out going radiation leads to very accurate loss values. Figure 2 shows a comparison between 3D FDTD and a Fourier Modal method [4]. The position of the light-line is seen to be around 1525nm in this case. Very low propagation loss is predicted above this wavelength (this is below the light-line in frequency terms) and this is the region where most waveguides are designed. This work is now going on to study the effect of surface roughness and disorder on these losses and is looking at structures with weak vertical confinement in material systems more suitable to implementing active components such as lasers and semiconductor optical amplifiers.

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## **Photonics Design Tools: Rising to Commercial and Technological Challenges**

*Trevor Benson, Phillip Sewell, Ana Vukovic, Ella Bekker, Svetlana Boriskina, Steve Greedy and Yaping Zhang, University of Nottingham*

### **Introduction**

Commercial success in the photonics marketplace requires that component and systems performance be maximized and product development time minimised. Meeting these twin goals can be significantly assisted by computer design and simulation, enabling a cost-effective, rapid evaluation of component

performance prior to manufacture. The demands placed upon the necessary simulation software continue to increase dramatically as 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 radiation be modelled to a high degree of accuracy. Here we present a non-mathematical overview of the photonics modeling capabilities within the George Green Institute for Electromagnetics Research (GGIEMR) at the University of Nottingham, and a few examples on how state-of-the-art simulation can satisfy the stringent requirements of component development. The research focus of the GGIEMR is on electromagnetic analysis and simulation techniques, applied as a generic discipline across a variety of frequencies and applications. Common 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, underpin much of our work.

## **Overview of our Methods**

Conventional time domain electromagnetic solvers such as TLM [1] and FD-TD [2] are extremely flexible and provide a rigorous numerical solution of Maxwell's equations. These tools can, in principle, be applied to a diverse range of materials and structures and so find use across the whole range of our research activities [3]. In the field of integrated photonics, we have for example applied TLM to the study of ring resonators, photonic crystals, and non-linear materials, [4]. However, these full wave time domain approaches require a direct discretization of the full spatial domain and their explicit nature necessitates the use of small time steps leading to long overall run times. This can be partially compensated for since domain decomposition techniques allow both FDTD and TLM to be parallelized with a high degree of speed-up, a fact attributable to the explicit nature of the algorithms. We are presently working on an unstructured meshing for the TLM method. This methodology ensures that the geometry of many practical structures can be described without staircasing errors, [5], and also enables fine features to be embedded within a coarser nu-

merical grid, another recurring theme across the whole range of our activities, [6].

To reduce the computational demand the Finite Difference Beam Propagation Method, FD-BPM, [7], replaces 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, with suitable boundary conditions, such as perfectly matched layers, 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. Even with these assumptions the demands FD-BPM makes on computer memory and processing times increase dramatically with the size of the numerical problem. The three-dimensional case, in particular, determines 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 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 [8, 9]. The discrete parameterization of the problem can also significantly affect the computational efficiency of any simulation. We have avoided this by developing structure-related coordinate schemes for frequency domain techniques, in which the all material boundaries align with coordinate lines in a parametric description of the geometry [10]. This provides substantial computational advantages for a given accuracy. Other important advances include finite difference schemes that allow arbitrary positioning of dielectric boundaries within a mesh [11], a technique we have further refined to enable fine structures such as quantum wells to be accurately modelled using a relatively large discretization [12]. The single-direction propagation assumption made by the BPM is clearly not acceptable for some situations and the method also struggles with the accurate modelling of wide angle scattering and coupling with evanescent fields. Reflective FD-BPM techniques are becoming

more sophisticated for discrete reflections and for two-dimensional problems, but they remain to be completely investigated for three-dimensional problems and fully assessed with continuous reflections.

Determining the modes of straight and curved waveguides still remains an essential activity when designing photonic systems. Real and imaginary distance BPM algorithms can be used for this purpose, or finite difference modal analysis techniques that generally exhibit the same advantages and disadvantages as the FD-BPM method. Despite the computational overheads, FD-based mode solvers are still widely used by us because of their flexibility, not only for studies of waveguides but also for components such as optical disks and micro-ring resonators. As an example, we consider a single mode Fibre on Glass (FOG) design. A coreless flurotellurite glass fibre of refractive index 1.842 on a flurotellurite glass substrate with a similar but lower refractive index of 1.841 was simulated at an operating wavelength 1.55  $\mu\text{m}$ . The elliptical rod has major and minor axis dimensions of 26  $\mu\text{m}$  and 15  $\mu\text{m}$  respectively (Fig.3a). Simulations show that the glass rod can provide single mode guiding when its bottom is embedded to a depth of approximately 2.5-5.5  $\mu\text{m}$  within the substrate. Fig.3b shows the field portrait of the mode supported at a wavelength of 1.55  $\mu\text{m}$  for an embedded depth of 4.5  $\mu\text{m}$ . All dimensions are in microns.

Notwithstanding the discussions above, the accurate simulation of a particular configuration may allow certain approximations to be made in what we refer to as a 'semi-analytical' approach. Within the remit of their physical approximations, semi-analytical analyses embrace general problems, and are extremely fast, accurate and robust. For example, when transverse refractive index contrasts are small, the Free Space Radiation Mode (FSRM) method [13] can be used (with no restriction on the index contrast in the direction of propagation). This approach proved invaluable in the analysis of buried waveguide structures such as semiconductor optical amplifiers. Similarly, the Spectral Index (SI) method [14] and Half Space Radiation Mode (HSRM) methods [15] apply to structures that employ a low-index (air) upper cladding. An SI-based mode-matching approach to simulating air-clad rib waveguide circuits was described in [16]. Also included in this classification are the plane-wave and localized-function methods that we have used to calculate the band gap structure of 2D photonic crystals and the modal properties of holey optical fibres. The calculations rely on evaluating the Fourier transform coefficients of the dielectric constant profile and we have derived a general formula for determining

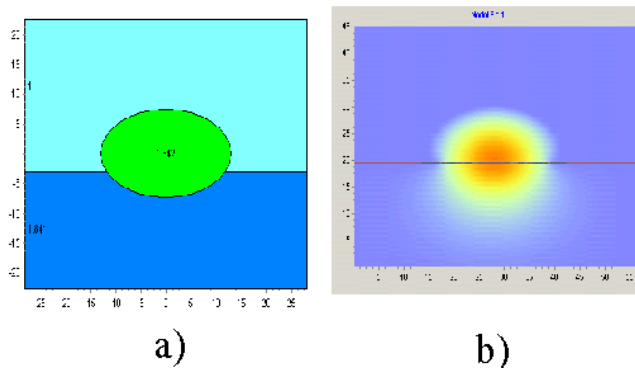


Figure 3: Fibre on Glass waveguide (a) and the field portrait of the single mode supported, calculated using a FD-based mode solver (b). All dimensions are in microns. The operating wavelength is 1.55  $\mu\text{m}$  and the embedded depth 4.5  $\mu\text{m}$ .

these coefficients for holes (rods) of arbitrary shape, [17]. Figure 4a shows the dielectric constant profile for a lattice of silicon rods in air. The lattice period is 2.3  $\mu\text{m}$ . Figure 4b,c shows the first and fifth H-polarised modes supported by this structure.

Under certain circumstances it has proven very useful to use a hybrid modelling approach. In [18] we described the modelling of fibre-to-chip coupling where a single-mode fibre was modelled using the FSRM method, and this coupled to an on-chip semiconductor rib waveguide that was modelled using the FD-BPM. The two methods were linked using an iterative procedure. The use of hybrid approaches to simulation is another unifying theme in the research work of the GGIEMR.

The use of optimization methods to automatically synthesize novel structures is also beneficial to optoelectronic design. By adaptively altering the accuracy of waveguide simulation during the optimization process, the synthesis of new designs can be speeded up. In our work, adaptive accuracy variation has been achieved by both altering the required numerical tolerance within a single method and by utilizing a hierarchy of differing methods. Our combination of optimization with, for example, adaptive semi-analytical simulations [19] is a

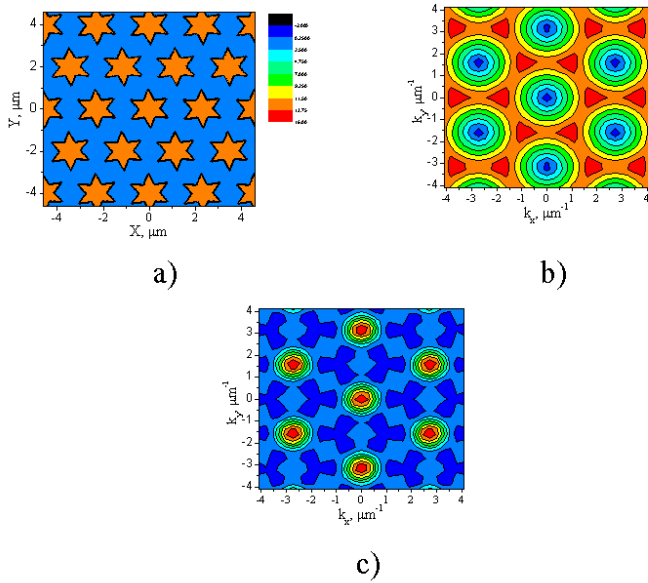


Figure 4: (a). Dielectric constant profile for a lattice of silicon rods in air. (b), (c) the first and fifth H-polarised modes supported by this structure

step towards the automatic CAD of optoelectronic components; knowledge of the solution accuracy within optimization enables synthesis to be undertaken to a user-defined accuracy. These methods can be extended to run effectively on parallel processors.

Integral Equation (IE) approaches show great promise for a wide class of problems. In our frequency domain version of this technique 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 [20]. We have also used them to (i) simulate the tuning of whispering-gallery mode (WGM) filter frequencies and coupling efficiencies for micro-ring resonators, designing-in intentional boundary imperfections to enhance Q-factors, reduce lasing thresholds, obtain directional light emission, and suppress parasitic modes, [21]; (ii) study surface roughness induced radiation loss and to estimate frequency shifts and loss-limited Q-factors in optical resonators, [22], and (iii) explore different micro-cavity shapes to design new structures with improved characteristics, [23]. We have also developed time domain IE techniques, discretised on an FD-like mesh [24-27]. 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. Hybrid tools combining numerical and integral equation approaches appear to be a fruitful way forward.

## **Conclusions**

Although full-wave time domain simulation techniques such as FDTD and TLM exist, many of today's simulation and design tools for optoelectronics involve approximations. Even then they are ultimately limited by computational resource. We have endeavoured to convey that a broad range of photonic devices and optical integrated circuits can be studied using a wide variety of numerical methods, many of these being developed at our Institute, and exploited in automated design optimization. The next generation of simulation software must aim to eliminate the limitations of these approaches, ideally solving the vector Helmholtz equation subject to open boundary conditions. It is tempting to propose that improvements in computing power will alleviate the problems

presently faced, but experience shows that today's urgent problem scales just, if not more, rapidly than available computing resources. Consequently, there is always going to be a significant role for techniques such as FD-BPM that improve this efficiency by making justifiable assumptions. However, the trend toward more widely available parallel computing facilities, and in particular, distributed computing will change the balance between the competing approaches.

## **Acknowledgements**

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## **Classic Techniques: Scattering from Cylinders**

*E. J. Grace and M. W. McCall*

We revisit a classic problem in electromagnetics, scattering of plane waves by infinite cylindrical rods. While conceptually quite simple, this "toy" nevertheless is instructive and demonstrates the principles and inherent limitations of similar, more sophisticated techniques. The solution of scattering problems is of great importance in many fields of optics. Many modern aspects of Photonics such as photonic crystals can be re-cast as complex scattering phenomena. Understanding how such techniques work, their implementation, range of validity and their pitfalls is of great importance. While the application of the technique described here has limited scope it is an excellent example of the principles behind many-body scattering problems.

The solution of scattering from an isolated cylinder has been known since Lord Raleigh. It is well understood and has been verified experimentally in a wide array of situations. When a set of such cylinders are placed together however the problem becomes considerably more involved. The scattering from one cylinder becomes an additional source to the incident wave of another cylinder. This mutual coupling of the scattered waves can be cast in the form of a large set of simultaneous equations which must be solved using the conventional techniques of linear algebra to yield the overall field as depicted in the figure on the front cover.

The size of the truncated matrix used to approximate the problem increases as the square of the number of cylinders and the number of coefficients. As a result the computational load to solve the full problem can explode quite dramatically.

We will outline an implementation of such a technique, essential tests that should be performed and where it can fail.

## Upcoming Computational Physics Group Events

### Computational Photonics

This meeting will be held in the Rankine building, room 408 at the University of Glasgow, on Wednesday, February 2<sup>nd</sup> 2005, from 1.20pm until 6pm.

Contact: D.Hutchings@elec.gla.ac.uk

### The 3<sup>rd</sup> Annual Computational Physics Thesis Prize

The Committee of the Institute of Physics Computational Group has endowed two annual prizes. £500 will be awarded to the author of the PhD thesis that contributes most strongly to the advancement of computational physics. Two runners-up will receive £250. There will be free group membership for 2005 for *all* entrants. The Committee will select the recipients and its remit will be very broad, in order to capture a broad spectrum of modelling activity.

- The deadline for applications is December 31<sup>st</sup>, 2004. The competition is open to all students whose PhD examination has taken place in 2004.
- The submission format is a 4 page (A4) abstract together with a citation (max. 500 words) from the PhD supervisor.

- The submission address is:  
DR M PROBERT  
DEPARTMENT OF PHYSICS  
UNIVERSITY OF YORK  
YORK, YO10 5DD

*Applicants must have carried out their thesis work at a University in the United Kingdom or the Republic of Ireland.*

The following were the winners of this year's competition:

- 1st place: David Walter
- 2nd place: Hans Fangohr
- 3rd place: Patrick Rinke and Emiliano Spezi

Given the high quality of the field we decided to make an extra award this time.

## Other Upcoming Meetings

### **The 11th International Conference on the Applications of Density Functional Theory in Chemistry and Physics**

The 11th International Conference on the Applications of Density Functional Theory in Chemistry and Physics (DFT2005) will be held September 11-15, 2005, in Geneva, Switzerland. This edition succeeds previous such biennial events organized in Brussels (2003), Madrid (2001), Rome (1999), Vienna (1997), ... The DFT2005 Conference will be devoted to both fundamental and applied aspects of Density Functional Theory (DFT) in Chemistry and Physics. The main topics covered by the Conference will be recent advances in:

- Fundamental aspects of DFT
- New exchange-correlation and kinetic energy functionals
- Conceptual DFT
- Weak interactions
- Magnetic properties
- Photochemical and photophysical properties
- Reactivity
- Materials
- Biosystems
- Dynamics

All the informations concerning Conference program, Committees, Registration, Accommodation, etc., may be found on the web site.

Web page: <http://DFT2005.unige.ch>