Photonic-crystal time-domain simulations using Wannier functions

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We present a Wannier-function-based time-domain method for photonic-crystal integrated optical circuits. In contrast to other approaches, this method allows one to trade CPU time against memory consumption and therefore is particularly well suited for the treatment of large-scale systems. As an illustration, we apply the method to the design of a photonic-crystal-based sensor, which utilizes a dual Mach–Zehnder–Fano interferometer. © 2011 Optical Society of America

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Over the past two decades, photonic crystals (PhCs) have developed into a mainstream research activity that reaches from fundamental research all the way to several applied areas [1]. With this increased importance comes a correspondingly increased demand for accurate computations concerning large-scale complex PhC-based integrated circuits.

General-purpose methods fail to exploit the underlying periodicity of the PhC backbone, and dedicated methods may exhibit distinct advantages. In particular, photonic Wannier functions (WFs) [2] provide a natural basis for the expansion of localized optical fields in PhC structures as they contain the full information about the underlying ideal PhC. In past years, this WF approach has evolved into a versatile tool for optimizing PhC structures via small-rank-update techniques [3] and WF-based sensitivity analyses [4]. In addition, a WF-based circuit theory allows us to treat large-scale systems [5]. All these achievements relate to frequency-domain methods, in which the WF method competes with a broad variety of other approaches, such as the plane-wave expansion. However, in spite of certain shortcomings, the finite-difference time-domain (FDTD) algorithm as, e.g., implemented in the software package MEEP [6] is virtually the only widely available method for time-domain simulations.

In this Letter, we begin to close this gap and develop a WF-based time-domain method that scales favorably (re- tense of memory consumption by fully taking advantage of the WFs’ properties. As an illustration, we apply our framework to the analysis of a dual Mach–Zehnder–Fano interferometer.

In this Letter, we begin to close this gap and develop a WF-based time-domain method that scales favorably (relative to FDTD) in terms of memory consumption by fully taking advantage of the WFs’ properties. As an illustration, we apply our framework to the analysis of a dual Mach–Zehnder–Fano interferometer (MZFI).

In this work, we restrict ourselves to $E$-polarized light in two-dimensional PhC systems, where the electric field propagates in the PhC’s plane of periodicity and is polarized along the transverse direction. Then, the electric field $E(\vec{r}) = (0, 0, E(\vec{r}))$ obeys the wave equation

$$\nabla^2 E(\vec{r}, t) = \frac{1}{c^2} \partial_t^2 \left( \epsilon_\rho(\vec{r}) + \delta \epsilon(\vec{r}) \right) E(\vec{r}, t).$$  

(1)

Here, $c$ is the vacuum speed of light and the entire PhC structure is described by the (real-valued) dielectric constant $\epsilon(\vec{r}) = \epsilon_\rho(\vec{r}) + \delta \epsilon(\vec{r})$, $\vec{r} = (x, y)$, which has been decomposed into two parts, $\epsilon_\rho(\vec{r})$ and $\delta \epsilon(\vec{r})$. They describe the ideal PhC and the deviations from perfect periodicity, respectively.

Next, we expand the electric field into a set of maximally localized WFs $W_\alpha(\vec{r})$ (see [2] for details on the generation and properties of WFs) with real-valued time-dependent coefficients $E_\alpha(t)$, according to $E(t, \vec{r}) = \sum_\alpha E_\alpha(t) W_\alpha(\vec{r})$. Here, $\alpha = (n, R)$ represents a compound index that labels the WFs via the band index $n$ and the home unit cell $R$. Upon inserting this expansion in the wave equation [Eq. (1)] and back-projecting onto the WF basis (Galerkin approach), we obtain

$$F_\alpha = \frac{1}{c} \partial_t E_\alpha, \quad \sum_\beta A_{\alpha\beta} E_\beta = \frac{1}{c} \partial_t \sum_\beta (C_{\alpha\beta} + D_{\alpha\beta}) F_\beta.$$  

(2)

In the semidiscrete equation [Eq. (2)], we have introduced the auxiliary field $F_\alpha$ that allows us to rewrite the second-order wave equation into a set of coupled first-order differential equations. In addition, we have used the matrices of WF coefficients [2]

$$A_{\alpha\beta} = \int_{\mathbb{R}^2} d^2 r W_\alpha^* (\vec{r}) \nabla^2 W_\beta (\vec{r}),$$

$$C_{\alpha\beta} = \int_{\mathbb{R}^2} d^2 r W_\alpha^* (\vec{r}) \epsilon_\rho (\vec{r}) W_\beta (\vec{r}),$$

$$D_{\alpha\beta} = \int_{\mathbb{R}^2} d^2 r W_\alpha^* (\vec{r}) \delta \epsilon (\vec{r}) W_\beta (\vec{r}).$$

(3)

To numerically evolve the fields, we replace the time derivatives in Eq. (2) by a backward-difference formula (BDF) [7] of second order according to

$$\partial_t E_\alpha^{(m)} = \frac{1}{\Delta t} (a_0 E_\alpha^{(m)} + a_1 E_\alpha^{(m-1)} + a_2 E_\alpha^{(m-2)}).$$

(4)

Here, $\Delta t$ is the time step and the coefficients $\{a_i\}$ define the specific form of the BDF. In addition, $E_\alpha^{(m)}$ denotes the state vector in the WF basis at time step $m$. Although higher-order BDF schemes exist, their stability could not be guaranteed without further knowledge of the spectrum of the system matrix. Finally, we recast the resulting

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system of linear equations (SLE) in an implicit update scheme, Eqs. (5a) and (5b):

\[ a_0 E_a^{(m)} = c \Delta t F_a^{(m)} - (a_1 E_a^{(m-1)} + a_2 E_a^{(m-2)}), \quad (5a) \]

\[
\sum_{\beta} \left( c^2 \Delta t^2 A_{\alpha \beta} + a_0^2 (C_{\alpha \beta} + D_{\alpha \beta}) \right) F_{\beta}^{(m)} \\
= c \Delta t \sum_{\beta} A_{\alpha \beta} (a_1 F_{\beta}^{(m-1)} + a_2 F_{\beta}^{(m-2)}) \\
- a_0 \sum_{\beta} (C_{\alpha \beta} + D_{\alpha \beta}) (a_1 F_{\beta}^{(m-1)} + a_2 F_{\beta}^{(m-2)}). \quad (5b) \]

As this SLE has to be solved in each time step, the overall performance of the method depends strongly on the properties of the matrices \( A, C, \) and \( D \). All of them are Hermitian and—due to the localization of the WFs—sparse. Owing to the translational symmetry of the underlying PhC, the matrices \( A, C, \) and \( D \) are of block-Toeplitz form [2]. Consequently, sparse LU-decomposition techniques, as, e.g., available in the PARDISO package [8], may be applied to systems of moderate numbers \( n \) of degrees of freedom. Unfortunately, this fails to take advantage of the matrices’ Toeplitz properties and fill-in during the factorization exhausts memory rather quickly.

For large-scale systems, we overcome these problems by using an iterative solver such as the BiCGStab(l) algorithm [9]. In particular, the change of the state vector from one time step to the next one is relatively small, so the fields at the previous time step provide an excellent starting point for the iteration. Thus, we require only about 20 iterations per time step, independent of the system size. This is tantamount to an effective \( O(n) \) scaling (see Fig. 1), and we attribute this behavior to the fact that the corresponding condition number of the SLE invariably saturates at a value of about 15. As a further advantage, BiCGStab(l) does not require the system matrix in explicit form. Instead, it is sufficient to provide only a matrix–vector product that may take full advantage of all properties of the matrices, in particular the Toeplitz structure. Through this, we can drastically reduce the memory consumption down to a level where the storage requirements are dominated by the state vectors \( E_a \) and \( F_a \). However, this memory efficiency comes at the expense of slowing down the code (see Fig. 1).

We have compared the performance of our WF-based time-domain (WFTD) approach with the software package MEEP. For this comparison, we have chosen a square array of silicon posts (lattice constant \( a \), dielectric constant \( \varepsilon_{Si} = 12 \), radius \( r = a/0.18a \)) in air. This PhC exhibits a complete photonic bandgap for frequencies between \( a/\lambda = 0.297 \) and \( a/\lambda = 0.442 \), where \( \lambda \) denotes the vacuum wavelength. The actual reference structure is a section of a W1 waveguide that consists of a row of missing posts along one of the crystallographic axes. The system is terminated via hard-wall boundary conditions at both ends. The number \( n \) of degrees of freedom is varied by changing the length of the waveguide. We have performed the WFTD computations by using nine WFs per PhC unit cell. Furthermore, we have neglected the coupling between unit cells that are separated by more than three lattice constants due to the strong localization of the WFs (see [2] for graphs of the WFs). With these parameters, WFTD computations for \( E \)-polarized radiation exhibit a relative accuracy of about \( 10^{-3} \) for physical quantities such as cavity mode frequencies.

In Fig. 1, we depict a comparison of the performance characteristics of our WFTD approach using different solvers for the associated SLE with MEEP computations of comparable accuracy (which are achieved for grid spacings below approximately \( a/50 \) according to our reference calculations). We find that all methods scale linearly in memory and CPU time with the number \( n \) of degrees of freedom. The memory-efficient implementation of WFTD is approximately a factor of 30 slower than FDTD but requires about 20 times less memory. This demonstrates how selecting an appropriate SLE solver allows one to trade execution speed for memory without affecting the overall accuracy.

At this point, we would like to note that optical nonlinearities can be treated straightforwardly within our framework by higher-rank tensors, such as

\[ D_{\alpha \beta \gamma}^{(NL)} = \int_{\mathbb{R}^2} d^2 r W_{\alpha} (\vec{r}) \chi^{(2)} (\vec{r}) W_{\beta} (\vec{r}) W_{\gamma} (\vec{r}). \]

for second-order nonlinear processes described by \( \chi^{(2)} (\vec{r}) \). The emerging system of nonlinear equations is then solved by Newton’s method. Furthermore, starting from the magnetic wave equation \( \nabla \times [\varepsilon (\vec{r}) \nabla \times H (\vec{r}, t)] = \frac{1}{\mu_0} \partial_t^2 H (\vec{r}, t) \), we can derive an explicit update scheme, which avoids solving a system of equations in each time step and, hence, provides a speed-up of approximately 1 order of magnitude. For linear computations, this approach is, therefore, very competitive to FDTD but does not straightforwardly allow us to treat nonlinear material response. The generalization toward three-dimensional (3D) comprises the availability of appropriate vector WFs and exchanging the integrals and operators in Eq. (3) with their 3D counterparts [10].

Open boundary conditions are difficult to realize for time-domain computations in PhCs, mainly because the periodically varying dielectric background reduces the performance of perfectly matched layers to first order. To date, adiabatic absorbers [11] exhibit the best performance and are easily incorporated into FDTD and WFTD.
frameworks by adding appropriate conductance terms to the wave equation.

As an illustration of our WFTD approach, we consider the dual MZFI [12] depicted in Fig. 2 that has been realized in our two-dimensional model PhC. We have terminated all waveguide ports with adiabatic absorbers with a length of 30 unit cells each (not shown in Fig. 2). The dual MZFI is illuminated with a broadband pulse and exhibits, in the absence of the add–drop filter, a very steep resonance (see left panel of Fig. 3) that can be shifted by slightly detuning one of the side-coupled cavities (open circle in square-shaped region). By adding a narrowband add–drop filter at the interferometer output, this shift of the resonance is translated into an amplitude change in the filter’s output channel (see right panel of Fig. 3). As a result, this circuit is very sensitive to slight changes in the refractive index of a single PhC unit cell and therefore implements a highly sensitive sensor principle.

In summary, we have developed an $O(n)$ WFTD method for the simulation of large-scale PhC circuits that allows us to flexibly trade CPU time for memory consumption. The method can be extended to treat optical nonlinearities and we have applied the method to the design of an integrated dual-MZFI-based sensor. Because of the multiresolution properties of the WFs [13], we anticipate a favorable scaling behavior for 3D PhC systems.

References