NON-CONFORMING FINITE ELEMENTS FOR WAVE SIMULATIONS ON LARGE GEOMETRIES

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Abstract

We present a new approach to simulate waves on large geometries. This method is based on newly developed Finite Elements, so-called Trigonometric Finite Wave Elements (TFWE), which are constructed by linear elements as well as by trigonometric functions such that the one-dimensional Helmholtz equation is exactly solved under certain conditions. In comparison with the Transfer Matrix Method the TFWE method offers as good results, but it can be extended to higher dimensions and it can be applied to time-dynamic problems. In two dimensions the TFWE are non-conforming elements. The analysis of TFWE shows that these elements approximate functions with certain oscillation properties more accurate than standard Finite Elements. Thus, a Finite Element discretization with TFWE leads to a smaller system of equations, which eases the solving process. Numerical results obtained by applying the TFWE method to the simulation of the wave equation for Distributed Feedback lasers are presented.

Derivation and Convergence of the Trigonometric Finite Wave Elements

Our aim is to solve the two-dimensional wave equation

$$-2\mathrm{i}\frac{k^2}{\omega}\frac{\partial E}{\partial t} = -\triangle E - k^2 E, \qquad (1)$$

which is coupled with a pair of partial differential equations for the carrier density called drift diffusion equation (see [1]):

$$\begin{aligned}\frac{\partial n_A}{\partial t} &= \nabla(D_A \nabla n_A) + \frac{n_B}{\tau_{cap}} - \frac{n_A}{\tau_{esc}} - r_{rec,A},\\ \frac{\partial n_B}{\partial t} &= \nabla(D_B \nabla n_B) + \eta_{i,leck}\frac{j_{inj}}{q d_B} - \frac{n_B}{\tau_{cap}}\frac{d_A}{d_B}\\ &\quad + \frac{n_A}{\tau_{esc}}\frac{d_A}{d_B} - r_{rec,B}.\end{aligned}$$

In standard simulations the above wave equation is reduced to the following stationary one-dimensional Helmholtz equation:

$$-\frac{\partial^2 E}{\partial x^2} - k^2 E = 0 \quad \text{on} \quad \Omega =]0, L[, \qquad (2)$$

where $k : \Omega \to \mathbb{R}$ is a piecewise constant function such that k is constant on the intervals $s_j =]p_{j-1}, p_j[$, $j = 1, ..., N$, $p_j = \frac{L}{N} j$ and $N \in \mathbb{N}$. Let us abbreviate $k_j = k\left(\frac{p_{j-1}+p_j}{2}\right)$.

A common and well-established method to solve the time-periodic Helmholtz equation (2) is the Transfer Matrix Method (TMM). The idea of this method is that the solutions of (2) are contained in $\mathcal{C}^1(\Omega)$ and that E has the form

$$E(z) = \alpha_j \exp(-\mathrm{i}k_j z) + \beta_j \exp(\mathrm{i}k_j z) \ \text{for} \ z \in s_j, \qquad (3)$$

where the coefficients α_j and β_j, $j \in \{1, ..., N\}$, have to satisfy two continuity equations resulting from the continuity of E and $\frac{dE}{dz}$ at the grid points p_j.

But general simulations require time-dependent, two-dimensional discretizations of (1), which cannot be obtained by the TMM. Standard Finite Element methods cannot be applied, as for resolving the wave appropriately, a huge amount of grid points is needed. Furthermore, the Beam Propagation Method is not suitable, as by this method it is very difficult to simulate internal reflections.

We propose a new Finite Element method, which provides for the one-dimensional Helmholtz equation as good results as the TMM, but which can be extended to two and three dimensions and can also be applied to time-dynamic calculations. The new method is similar to the method described in [2], however, the two-wave ansatz cannot be applied to simulate internal reflections, which appear in Distributed Feedback (DFB) lasers. Let us explain the new method in one dimension. The idea is to construct new basis functions by multiplying $v^h_{p_j}(z)$ with trigonometric cosine and sine functions, which approximate the behavior of an oscillating wave. In case of linear Finite Elements, $v^h_{p_j}(z)$ denotes the nodal basis function, which is 1 at p_j and 0 at all other grid points $p_i,\ i \neq j$, where $h = \frac{L}{N}$ is the mesh size of the discretization grid. Now we can define the following basis functions at grid point p_j:

$$B^{\cos}_j(z) := \cos\left(k(z)(z - p_j)\right) v^h_{p_j}(z),$$

$$B^{\sin}_j(z) := \sin\left(k(z)(z - p_j)\right) v^h_{p_j}(z),$$

and

$$B_j^{mix}(z) := mix\big(k(z)(z-p_j)\big)v_{p_j}^h(z)$$
$$:= \begin{cases} -\sin\big(k_j(z-p_j)\big)v_{p_j}^h(z) & \text{if } z \le p_j \\ \sin\big(k_{j+1}(z-p_j)\big)v_{p_j}^h(z) & \text{if } z > p_j. \end{cases}$$

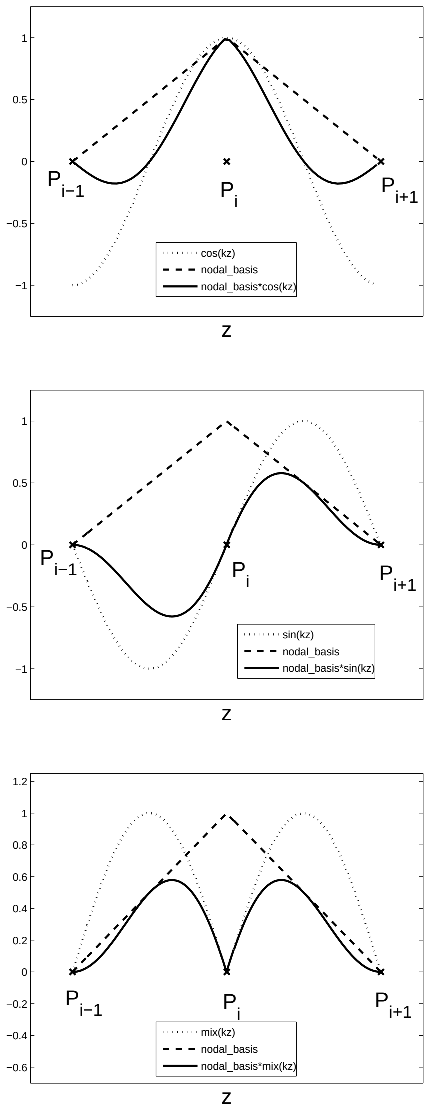

Figure 1: Cosine, Sine, and Mixed Basis Function

These basis functions are called Trigonometric Finite Wave Elements and span the space

$$V_h := \Big\{ u \in H^1(\Omega) \quad \Big| \quad u(z) = \sum_{j=0}^{N} a_j B_j^{\cos}(z) + b_j B_j^{\sin}(z) + c_j B_j^{mix}(z), \quad a_j, b_j, c_j \in \mathbb{C},\ c_0 = c_N = 0 \Big\}.$$

Introducing suitable boundary conditions, which can be handled by TMM as well as by TFWE, we can show that the solutions (3) of the one-dimensional Helmholtz equation derived by the TMM are contained in the space spanned by the TFWE (see [3]).

An important advantage of the TFWE method in comparison with the TMM is that it can be applied to general wave number coefficients k and in two and more dimensions:

Let $\Omega =]0, L[\times]0, W[$ and let $k \in L^\infty(\Omega)$ such that k is a continuous function on each subdomain $]H(j-1), Hj[\times[0, W]$, $j = 1, ..., m$, where $H = \frac{L}{m}$ and $m \in \mathbb{N}$. Now, we introduce two meshsizes $h_x = \frac{L}{N_x}$ and $h_y = \frac{W}{N_y}$ and the meshsize tuple $\boldsymbol{h} := (h_x, h_y)$, where $N_x = nm$, $n \in \mathbb{N}$, and $N_y \in \mathbb{N}$. This leads to the grid points $p_{ij} := (x_i, y_j) := (ih_x, jh_y)$ and grid cells $r_{ij} = [x_{i-1}, x_i]\times]y_{j-1}, y_j[$, $i \in \{1, ..., N_x\}$, $j \in \{1, ..., N_y\}$, such that $\bigcup_{j=1}^{N_y}\bigcup_{i=1}^{N_x} \bar{r}_{ij} = \Omega$.

Now, let $k_{\boldsymbol{h}}$ be the interpolant of k at the midpoints of each cell r_{ij} such that $k_{\boldsymbol{h}}$ is piecewise constant on $\mathring{r}_{ij}$. This means that $k_{\boldsymbol{h}}(x, y) := k_{ij} := k(\frac{x_{i-1}+x_i}{2}, \frac{y_{j-1}+y_j}{2})$ for every $(x, y) \in \mathring{r}_{ij}$. We construct the TFWE in two dimensions by taking the tensor product of the one-dimensional TFWE and the linear nodal basis functions in y-direction. Thus, we get the following basis functions at grid point p_{ij}:

$$B_{ij}^{\cos}(x, y) := \cos\big(k_{\boldsymbol{h}}(x, y)(x - x_i)\big)v_{x_i}^{h_x}(x)v_{y_j}^{h_y}(y),$$

$$B_{ij}^{\sin}(x, y) := \sin\big(k_{\boldsymbol{h}}(x, y)(x - x_i)\big)v_{x_i}^{h_x}(x)v_{y_j}^{h_y}(y),$$

and

$$B_{ij}^{mix}(x, y) := mix\big(k_{\boldsymbol{h}}(x, y)(x - x_i)\big)v_{x_i}^{h_x}(x)v_{y_j}^{h_y}(y),$$

where

$$mix\big(k_{\boldsymbol{h}}(x, y)(x - x_i)\big) = \begin{cases} -\sin\big(k_{\boldsymbol{h}}(x, y)(x - x_i)\big) & \text{if } x \le x_i \\ \sin\big(k_{\boldsymbol{h}}(x, y)(x - x_i)\big) & \text{if } x > x_i. \end{cases}$$

As these basis functions are discontinuous in y-direction, let us define the space $\Omega_{\boldsymbol{h}} := \bigcup_{i=1}^{N_x}\bigcup_{j=1}^{N_y} r_{ij}$ and the corresponding seminorm

$$|u|_{H^1(\Omega_{\boldsymbol{h}})} := \left(\sum_{i=1}^{N_x}\sum_{j=1}^{N_y}\int_{r_{ij}} \left|\frac{\partial u}{\partial x}(x, y)\right|^2 + \left|\frac{\partial u}{\partial y}(x, y)\right|^2 d(x, y) \right)^{\frac{1}{2}}.$$

Then these TFWE span the space

$$V_{\boldsymbol{h}}^{2D} := \Big\{ u \in H^1(\Omega_{\boldsymbol{h}}) \Big| \; u(x,y) = \\ = \sum_{j=0}^{N_y} \sum_{i=0}^{N_x} a_{ij} B_{ij}^{\cos}(x,y) + b_{ij} B_{ij}^{\sin}(x,y) \\ + c_{ij} B_{ij}^{mix}(x,y) \quad \forall (x,y) \in \Omega, \\ a_{ij}, b_{ij}, c_{ij} \in \mathbb{C}, \; c_{0j} = c_{N_x j} = 0 \Big\}.$$

Remark. As $H^1(\Omega_{\boldsymbol{h}}) \nsubseteq H^1(\Omega)$, the Finite Element space $V_{\boldsymbol{h}}^{2D} \nsubseteq H^1(\Omega)$ is non-conforming.

Let us consider the following weak problem derived from a time discretization of (1):

Find $u \in H^1(\Omega)$ *such that* $a(u,v) = \boldsymbol{f}(v), \;\forall v \in H^1(\Omega)$, *where*

$$a(u,v) := \int_\Omega \big(\nabla u(x,y) \nabla \bar{v}(x,y) - k^2 u(x,y) \bar{v}(x,y) \\ + \mathrm{i}\beta u(x,y) \bar{v}(x,y) \big) d(x,y)$$

and $\beta > 0$.

Let us assume that the solution u satisfies the Oscillation Assumption:

Assumption 1 (Oscillation Assumption) *Let* $u \in H^2(\Omega_{\boldsymbol{h}})$ *be a function oscillating with an angular frequency* ω *similar to* ck, *where* c *is the velocity of light. In mathematical notation this means that* u *can be written as*

$$u = u^+ \exp(\mathrm{i}kx) + u^- \exp(-\mathrm{i}kx),$$

where $u^+ \exp(\mathrm{i}kx) \in C(\Omega)$, $u^- \exp(-\mathrm{i}kx) \in C(\Omega)$, $|\frac{d^2u^+}{dx^2}|_{L^2(\hat{\Omega}_{\boldsymbol{h}})} \ll |\frac{d^2 u}{dx^2}|_{L^2(\Omega)}$, *and* $|\frac{d^2u^-}{dx^2}|_{L^2(\hat{\Omega}_{\boldsymbol{h}})} \ll |\frac{d^2 u}{dx^2}|_{L^2(\Omega)}$.

Herein, $|u|_{X(\hat{\Omega}_{\boldsymbol{h}})}$ defines the X-norm of the space $\hat{\Omega}_{\boldsymbol{h}} := \bigcup_{i=1}^{N_x} \bigcup_{j=1}^{N_y} \mathring{r}_{ij}$.

Theorem 1 *Let* $u \in H^2(\Omega)$ *satisfy Assumption 1. Then, there exists a constant* c *independent of* $h := \max\{h_x, h_y\}$ *such that*

$$|u - u_{\boldsymbol{h}}|_{H^1(\Omega_{\boldsymbol{h}})} \leq ch \Big(|u^+|_{H^2(\hat{\Omega}_{\boldsymbol{h}})} + |u^-|_{H^2(\hat{\Omega}_{\boldsymbol{h}})} \Big)$$

holds.

The proof of this theorem can be found in [3].

Application and Numerical Results

Finally, we present numerical simulation results for the optical wave in DFB lasers achieved by the TFWE method. We solved the weak form of (1) numerically, where laser resonators of different size emitting at wavelength $1300nm$ were considered. In Figure 2 a laser resonator of size $30\mu m \times 130\mu m$ with a small stripe width of size $2\mu m$ was chosen, whereas in Figure 3 a laser resonator of size $120\mu m \times 130\mu m$ with a large stripe width of size $40\mu m$ is shown. Herein, the photon density n is defined by $n = \frac{\epsilon}{2\hbar\omega}(|E|^2)$.

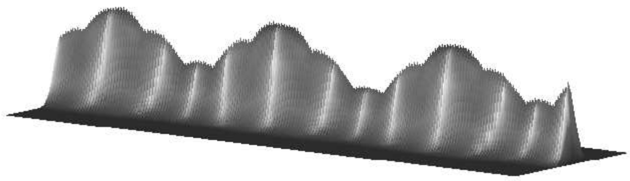

Figure 2: Photon density n: mode of first order is achieved by a small stripe width s

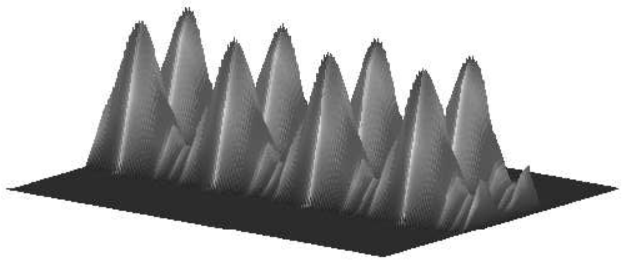

Figure 3: Photon density n: mode of higher order due to a “large” stripe width s

References

[1] G. Steinle, “Neuartige monolithische InAlGaAsN Vertikallaserdioden: langwellige Emission bei $1.3\mu m$, Monitordiodenintegration, Modellierung”, Ph.D. thesis, Institute of Optoelectronics, Ulm University, Germany, 2002.

[2] K. Altmann, C. Pflaum, and D. Seider, “Three-Dimensional Finite Element Computation of Laser Cavity Eigenmodes”, Applied Optics-LPE, vol. 43, n° 9, pp. 1892-1901, 2004.

[3] B. Heubeck, C. Pflaum, and G. Steinle, “New Finite Elements for Large-Scale Simulation of Optical Waves”, in preparation.