INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 11, Number 2, Pages 303–314



# ON COMPACT HIGH ORDER FINITE DIFFERENCE SCHEMES FOR LINEAR SCHRÖDINGER PROBLEM ON NON-UNIFORM MESHES

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(Communicated by F.J. Gaspar)

*This paper is dedicated to Prof. Francisco Lisbona*

**Abstract.** In the present paper a general technique is developed for construction of compact high-order finite difference schemes to approximate Schrödinger problems on nonuniform meshes. Conservation of the finite difference schemes is investigated. The same technique is applied to construct compact high-order approximations of the Robin and Szeftel type boundary conditions. Results of computational experiments are presented.

**Key words.** finite-difference schemes, high-order approximation, compact scheme, Schrödinger equation, Szeftel type boundary conditions.

## 1. Introduction

High power high brightness edge-emitting semiconductor lasers and optical amplifiers are compact devices and they can serve a key role in different laser technologies such as free space communication [3], optical frequency conversion [11], printing, marking materials processing [16], or pumping fiber amplifiers [13].

To simulate the generation and/or propagation of the optical fields along the cavity of the considered device one can use a 2+1 dimensional system of PDEs which is based on the traveling wave (TW) equations for slowly varying in time longitudinally counter-propagating and laterally diffracted complex optical fields $E^{\pm}(z,x,t)$ [2], which are nonlinearly coupled to the linear ODEs for the complex induced polarization functions $p^{\pm}(z,x,t)$ and to the diffusion equation for the real carrier density $N(z,x,t)$ [17]:

$$\frac{\partial E^{\pm}}{\partial t} \pm \frac{\partial E^{\pm}}{\partial z} = -\frac{i}{2}\frac{\partial^2 E^{\pm}}{\partial x^2} - i\beta(N,|E^{\pm}|^2)E^{\pm} - i\kappa^{\mp}E^{\mp} - g_p(E^{\pm}-p^{\pm}),$$
$$\frac{\partial p^{\pm}}{\partial t} = i\omega_p p^{\pm} + \gamma_p\big(E^{\pm}-p^{\pm}\big),\ \frac{1}{\mu}\frac{\partial N}{\partial t} = \frac{\partial}{\partial x}\Big(D\frac{\partial N}{\partial x}\Big) + \Re e\,\mathcal{N}\big(N,E^{\pm},p^{\pm}\big)\,.$$

Here, $t \in \mathbb{R}_+$, $z \in [0,L]$ and $x \in \mathbb{R}$ denote temporal, longitudinal and lateral coordinates, respectively. Functions $\beta$, $\mathcal{N}$ and parameters $g_p$, $\kappa^{\mp}$, $\omega_p$, $\gamma_p$, $D$, $\mu$ represent the propagation factor, injected current and nonlinear carrier recombination, Lorentzian gain amplitude, field coupling coefficient, gain peak detuning, Lorentzian half-width at half maximum, carrier diffusion coefficient, photon/carrier life time relation, respectively. Optical field functions $E^{\pm}$ satisfy the following reflection-injection conditions at the longitudinal boundaries of the domain:

$$E^{+}(0,x,t) = r_0(x)E^{-}(0,x,t) + a_0(x,t),$$
$$E^{-}(L,x,t) = r_L(x)E^{+}(L,x,t) + a_L(x,t).$$

Received by the editors November 14, 2012 and, in revised form, May 24, 2013.
2000 *Mathematics Subject Classification.* 65M06.

The initial conditions (if properly stated) are not very important, since after some transients the simulated trajectories approach one of the existing stable attractors.

A large scale system implied by a discretization of the computational domain and an appropriate approximation of artificially imposed lateral boundary conditions can be solved effectively with the help of parallel computing [17, 4, 10]. However, for the precise dynamic simulations of long and broad devices and tuning/optimization of the model with respect to one or several parameters, a further speedup of computations is still desired.

Since, in general, the carrier dynamics is slow ($0 < \mu \ll 1$), and in the most cases the polarization equations have only a small impact on the overall dynamics of the optical fields ($0 \leq g_p/\gamma_p \ll 1$), a proper construction of numerical schemes for the diffractive field equations plays a decisive role. Here we note, that for the temporarily fixed distribution of the propagation factor $\beta$, neglected polarization and absent coupling between counter-propagating fields (vanishing distributed coupling $\kappa^{\pm} = 0$ as well as field reflectivities at the longitudinal boundaries $r_0 = r_L = 0$), the equation for the forward (backward) propagating field on the characteristic lines $t - z = t_0$ (or $t - (L - z) = t_0$) is given by a linear 1+1 dimensional Schrödinger equation

$$\frac{\partial u}{\partial \nu} = -\frac{i}{2}\frac{\partial^2 u}{\partial x^2} - i\mathcal{B}(\nu, x)u,$$

where the field $u(\nu, x) = E^+(z, x, t)$ (or $u(\nu, x) = E^-(L - z, x, t)$), and the initial condition $u(0, x)$ is defined by the optical injection function $a_0(x, t)$ (or $a_L(x, t)$). Thus, a construction of the effective numerical schemes for the full model is closely related to the construction of the schemes for above given linear Schrödinger problem. One of the main challenges in this case is an implementation of the appropriate boundary conditions (BCs) [1]. In our previous paper [6] we have investigated the performance of the standard Crank-Nicolson scheme supplemented with the exact discrete transparent boundary conditions (DTBCs) [8], with the approximate DTBCs suggested by Szeftel [18] as well as with simple Dirichlet boundary conditions.

The main goal of the present paper is to develop a general technique for construction of compact high-order finite difference schemes for approximation of Schrödinger problems on nonuniform meshes. All these schemes can be of practical interest when dealing with broad lasers having a relatively high regularity of transversal heterostructures. In this case, due to enhanced spatial approximation precision, we can use a relatively sparse mesh in the transversal spatial direction, and, nevertheless, obtain the numerical solutions with a required precision. We note that in the case of uniform meshes, for the compact high-order finite difference scheme the corresponding exact DTBCs are derived in [12, 15]. We note that using the same ideas exact DTBCs can be constructed for the compact high-order finite difference schemes on non-uniform meshes, but such BCs are non-local in time and are not very efficient for applied problems described above.

The rest of the paper is organized as follows. In Section 2 we construct compact finite difference schemes on uniform and nonuniform meshes. On uniform mesh this high-order finite difference scheme coincides with the Numerov approximation. The conservation laws of the constructed finite difference schemes are investigated. For non-uniform meshes these laws can be violated due to non-symmetrical approximation of the source terms.

In Section 3, by using the technique from the previous section, we construct compact high-order approximations of the Robin type BCs, which can be interpreted