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**Construction of Discrete Transparent
Boundary Conditions for
Schrödinger-Type Equations**

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Abstract

We present a general technique for constructing nonlocal transparent boundary conditions for time-discretized one-dimensional Schrödinger type equations. The main tool of construction is the discrete counterpart to Mikusiński's continuous algebraic operator approach. Existing techniques are simplified and generalized. Both adaptive time-steps and time-dependent exterior potentials are taken into account.

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1 Introduction

The paper deals with the construction of transparent boundary conditions for discretized Schrödinger-type equations. Let the continuous partial differential equation be given as

$$\begin{aligned}\partial_t u &= -\frac{i}{c} (\partial_x^2 u + V(x, t)u), \quad x \in \mathbf{R}, t > 0 \\ u(x, 0) &= u_0.\end{aligned}\tag{1}$$

Here c is a real constant and $V(x, t)$ denotes the potential to be specified later. Prototypes of this equation are the Schrödinger equation for an electron with mass m_0

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m_0}\partial_x^2\Psi + V(x, t)\Psi$$

and Fresnel's equation for the evolution of a paraxial electrical field E along the z -direction in a Cartesian coordinate system

$$2in_0k_0\partial_z E = \partial_x^2 E + (n^2(x) - n_0^2)k_0^2 E.$$

We consider the evolution equation (1) in the infinite domain $\Omega = \{x, t \in \mathbf{R} \mid t > 0\}$. Further, we assume that the initial function $u_0(x)$ has support only in a finite interval and a finite norm $\|u_0(x)\|_{L^2}$. Then we expect from the conservation properties of (1) that $u(x, t)$ vanishes for $x \rightarrow \pm\infty$ at any time $t > 0$. Thus, imposing Dirichlet boundary conditions at infinity, we are able to solve the equation. From a practical point of view, however, one is often interested in studying the evolution of the solution just in the surrounding of some object. Therefore the infinite domain Ω is decomposed into an interior domain Ω_i containing the object of interest and its complement with respect to the whole domain Ω . In our 1D-case we define $\Omega_l = \{x, t \in \mathbf{R} \mid x_1 \leq x \leq x_r, t > 0\}$, and the exterior domain consists of the two domains $\Omega_l = \{x, t \in \mathbf{R} \mid x \leq x_1, t > 0\}$ and $\Omega_r = \{x, t \in \mathbf{R} \mid x \geq x_r, t > 0\}$, for the left and right semi-infinite sub-domains, respectively. The aim of this paper is to supply methods which transform the zero-boundary conditions at infinity to the boundary conditions at the boundaries of the interior domain. Besides the discrete approach, which we emphasize in this paper, there are a large number of other methods.

Artificially absorbing layers. From the physical point of view, it is a natural to modify the potential function in the exterior domain such that an artificial absorption is generated. The parameters describing the absorber-function have to be adjusted such that backward diffraction from the absorber is small over a prescribed spectral range (e. g. KOSLOFF and KOSLOFF [7] or YEVICK [12]). The main advantage of such an approach, as has been

remarked by a large number of authors, is its simplicity for two and three-dimensional problems.

A rather recent approach due to BÉRENGER [3], the perfectly matched layer (PML) method, not only changes the potential function in the exterior domains but the whole equation is converted into a different one, which coincides with the original equation only at the boundaries itself. The method turned out to be very efficient for many problems. Here we have the same simple formulation for 2D and 3D problems but also the same problem in finding the best choice of parameters for given task. A study of the PML-technique with respect to Schrödinger-type equations in the context of optical beam propagation may be found in [13].

Local boundary conditions. A second class of methods is obtained by employing the calculus of pseudo-differential operators. The main steps to derive such boundary conditions are the following. At first, the partial differential equation is converted to a second-order differential equation in space by Laplace transforming in time. The transformed differential equation is then solved allowing only for decaying modes in the exterior domains. In case of higher space-dimensions (≥ 2) one obtains local approximations in space using the theory of pseudo-differential operators. After transforming back into the time-domain the resulting transparent boundary conditions in general become local in space but nonlocal in time. To avoid the additional costs in terms of computer resources due to the non-locality in time, the dispersion relation between time- and space-variables may be rational approximated in the dual domain. This construction scheme has been successfully applied by a number of authors. Following the pioneering work of ENGQUIST and MAJDA [4] on hyperbolic equations, advanced approximation techniques have been proposed for mixed parabolic-hyperbolic systems (HALPERN, [6]) or parabolic equations (HAGSTROM, [5]).

Nonlocal boundary conditions. However, there are a number of problems acting very sensitive with respect to the magnitude of the reflected field. In such cases the inherent non-locality of the boundary conditions has to be taken into account. The two main approaches for constructing boundary conditions for the discretized evolution equation are, first, solving the continuous exterior problem first by means of a Green's function technique and then discretizing the continuous boundary condition with respect to time, as suggested by BASKAKOV and POPOV [2]. However, such approaches may lead to numerical instabilities. A theoretical study may be found in [8], where it is shown that numerical stability, even in the case of uniform discretization both in time (with time-step Δt) and space (with space-step Δx), is given only in disjoint intervals for $\Delta t/\Delta x^2$. Alternatively, the problem of finding boundary conditions for the discretized equation, can

be consistently formulated for discrete time. In this manner, ARNOLD [1] compose a boundary condition which incorporates both a uniform space and a uniform time discretization. Besides the uniformity of discretization, the time-independency of the potential in the exterior domain is an essential prerequisite. The key point in his approach is that the uniform space discretization of the interior domain is continued to the exterior domain as well. In contrast, the approach [10] supposes a given, possible nonuniform, time-discretization and an arbitrary inner space-discretization. The space-variable in the exterior domain is not discretized. Additionally, the outer potential may be a function of time. We will label this approach the semi-discrete method. In [11] we have shown that our semi-discrete method covers ARNOLD's fully discrete method. Further, it turned out that the approach [11] supplies the desired boundary conditions in a very clear and concise manner. Therefore the following is based in parts on that work.

In the sequel, we will generalize this technique to get rid off the unnatural restriction to uniform time-steps and time-independent exterior potentials. The method is developed in complete analogy to MIKUSŃSKI's [9] operational calculus. The difference is that MIKUSŃSKI considered an algebra based on continuous, complex valued functions over a semi-infinite time-interval, whereas our basic elements are semi-infinite sequences of complex numbers.

Let us rewrite (1) as

$$\begin{aligned}\partial_t u &= f(u, t), \quad (x, t) \in \Omega \\ \lim_{x \rightarrow \pm\infty} u(x, t) &= 0.\end{aligned}$$

To solve this equation numerically, we apply the implicit one-step discretization

$$\begin{aligned}u_{i+1} - u_i &= \tau f(\theta u_{i+1} + (1 - \theta)u_i, t_i + \theta\tau) \\ \tau &= t_{i+1} - t_i, \quad i = 0, 1, \dots \\ 0 &< \theta \leq 1.\end{aligned}$$

Using the definition of $f(u, t)$ from (1), we find

$$u_{i+1} - u_i = -i\frac{\tau}{c} \left((\partial_x^2 + V)(\theta u_{i+1} + (1 - \theta)u_i) \right). \quad (2)$$

By rearranging the terms we obtain

$$\begin{aligned}\partial_x^2 u_{i+1} - \lambda^2 u_{i+1} &= -\Theta \partial_x^2 u_i + \kappa^2 u_i. \\ \Theta &= \frac{1 - \theta}{\theta} \\ \lambda^2(x, t_i + \theta\tau) &= \frac{ic}{\tau\theta} - V(x, t_i + \theta\tau) \\ \kappa^2(x, t_i + \theta\tau) &= -\frac{ic}{\tau\theta} - \Theta V(x, t_i + \theta\tau).\end{aligned} \quad (3)$$

We now seek solutions u_i , $i \geq 1$ of (3) that vanish at infinity. We focus here on obtaining an exterior solution which enables the boundary conditions to be constructed, independently of the numerical method employed to solve the interior problem. For this purpose, we fix the right boundary at $x_t = 0$, $t > 0$ and search for solutions $u_i(x)$, $i \geq 1$, $x \geq 0$ in the right exterior domain. These exterior solutions have to obey the boundary condition at infinity

$$\lim_{x \rightarrow \infty} u_i(x) = 0, \quad i \geq 1. \quad (4)$$

Continuous treatment of the space coordinate. In the semi-discretized equation (2) the space-variable x appears as continuous variable. Therefore (2) forms a sequence of ordinary differential equations. A convenient way to solve such sequences is to convert them into an algebraic system by means of the Laplace transformation. With

$$U_i(p) = \mathcal{L}u_i(x) = \int_0^\infty e^{-px} u_i(x) dx, \quad p \in \mathbf{C}, \quad \Re(p) > 0,$$

we find the equivalent transformed system to

$$(p^2 - \lambda_{i+1}^2) U_{i+1}(p) + (\Theta p^2 - \kappa_{i+1}^2) U_i(p) = pu_{i+1}(0) + \partial_x u_{i+1}|_{x=0} + \Theta(pu_i(0) + \partial_x u_i|_{x=0}). \quad (5)$$

Discrete treatment of the space coordinate. The alternative idea is to consider a uniformly discretized space. That is, we associate the solution points at the i th propagation step with physical locations according to the formula

$$u_i^{(j)} = u_i(j \cdot h), \quad j \geq -1, \quad i \geq 0.$$

Here $u_i^{(-1)}$ is the rightmost inner value in Ω_i while u_i^0 is located on the boundary between the internal and the right external region. The equation corresponding to (5) is obtained by introducing the sequences

$$\begin{aligned} \mathbf{u}_i &= \{u_i^{(0)}, u_i^{(1)}, u_i^{(2)}, \dots\} \\ \mathbf{u}_i^+ &= \{u_i^{(1)}, u_i^{(2)}, u_i^{(3)}, \dots\} \\ \mathbf{u}_i^- &= \{u_i^{(-1)}, u_i^{(0)}, u_i^{(1)}, \dots\}, \end{aligned}$$

with Z -transforms

$$\begin{aligned} \mathcal{U}_i &= \mathcal{Z}\mathbf{u}_i = u_i^{(0)} + \frac{1}{z}u_i^{(1)} + \frac{1}{z^2}u_i^{(2)} + \dots \\ \mathcal{U}_i^+ &= \mathcal{Z}\mathbf{u}_i^+ = u_i^{(1)} + \frac{1}{z}u_i^{(2)} + \frac{1}{z^2}u_i^{(3)} + \dots \\ \mathcal{U}_i^- &= \mathcal{Z}\mathbf{u}_i^- = u_i^{(-1)} + \frac{1}{z}u_i^{(0)} + \frac{1}{z^2}u_i^{(1)} + \dots \end{aligned}$$

By Z-transforming the finite-difference form of (3) and taking into account the relations between $\mathcal{U}_i$, $\mathcal{U}_i^+$, and $\mathcal{U}_i^-$, we obtain the discrete counterpart to (5)

$$\left(z - (2 + h^2\lambda^2) + \frac{1}{z}\right)\mathcal{U}_{i+1}(z) + \Theta\left(z - (2 + h^2\kappa^2/\Theta) + \frac{1}{z}\right)\mathcal{U}_i(z) = u_{i+1}^{(-1)} - zu_{i+1}^{(0)} + \Theta(u_i^{(-1)} - zu_i^{(0)}) \quad (6)$$

Comparing (5) and (6) we do not find any qualitative difference in the structure of these equations with respect to the time-evolution. The only difference is that the factors before $\mathcal{U}_{i+1}$ and $\mathcal{U}_i$ are slightly more involved. Based on this similarity, we restrict all of our following considerations to (5). The corresponding results for (6) are obtained in complete analogy.

2 Mikusiński's operational calculus

Let $\{U\}$ be the sequence of the complex valued functions $\{U_0(p), U_1(p), \dots\}$, which appear as solutions of (5). The key-point in our analysis of recursively defined functions U_i is to consider relations between objects of type $\{U\}$ instead of individual functions U_i . We aim to replace (5) by an algebraic relation between sequences. In order to do this we have to establish the operations of *addition* and *multiplication* and their inverse operations. We do this in complete analogy to MIKUSIŃSKI's operational calculus.

Let $\mathcal{C}$ be the set of all complex-valued, discrete functions $\{U\} = \{U_0, U_1, U_2, \dots\}$ with $U_i \in \mathbf{C}$. When possible, we use the notation U instead of $\{U\}$. The sum of two elements $U, V \in \mathcal{C}$ is defined as

$$U + V = \{U_0 + V_0, U_1 + V_1, \dots\}.$$

The multiplication is defined as discrete convolution via

$$UV = \{G_0, G_1, \dots\}, \quad \text{with} \quad G_i = \sum_{j=0}^i U_{i-j}V_j.$$

From these definitions we find $UV = VU$, $U(VW) = (UV)W$ and $U(V + W) = UV + UW$. Hence, $\mathcal{C}$ is a commutative ring. Further we know that for $U, V \in \mathcal{C}$ the equation $U \cdot V = 0$ implies either $U = 0$ or $V = 0$ or both, where 0 denotes $\{0, 0, \dots\}$. Hence, we can extend the ring $\mathcal{C}$ to the ring of *fractions* $\mathcal{C}_q$

$$\mathcal{C}_q = \left\{ \frac{U}{V} \mid U \in \mathcal{C}, V \in \mathcal{C} \setminus \{0\} \right\}.$$

Two fractions U/V and U'/V' are defined to be equal $U/V = U'/V'$ if and only if $UV' = VU'$. The addition and multiplication of two fractions are

defined by

$$\frac{U}{V} + \frac{U'}{V'} = \frac{UV' + VU'}{VV'} \quad \text{and} \quad \frac{U}{V} \cdot \frac{U'}{V'} = \frac{UU'}{VV'},$$

respectively. Some special elements of $\mathcal{C}_q$ are labeled with their own symbols. The multiplication with a number $a \in \mathbf{C}$ is realized via the multiplication operator $[a]$

$$[a] = \{a, 0, 0, \dots\}.$$

If no ambiguity occurs, we write simply $[a]\{U\} = aU$. Further, we label the shift-operator with the symbol s

$$s = \{0, 1, 0, \dots\},$$

and find $s \cdot s = s^2 = \{0, 0, 1, 0, \dots\}$ etc. A general mapping $\mathbf{A} : \mathcal{C} \longrightarrow \mathcal{C}$ with infinite matrices $\mathbf{A} = (a_{i,j})_{i,j=0,\dots,\infty}$ maps U into V , $U \mapsto V = \mathbf{A}U$, by a matrix-vector-multiplication $V_i = \sum_{j=0}^{\infty} a_{i,j}U_j$.

3 Construction of discrete transparent boundary conditions

Now we are able to reformulate our original problem (5) using the algebraic operator method. In order to do this, we rewrite the sequence (5) into a matrix equation with infinite dimensional matrices.

$$\left[p^2 \begin{pmatrix} 1 & & & & \\ \Theta & \ddots & & & \\ & \ddots & 1 & & \\ & & \Theta & 1 & \\ & & & \ddots & \ddots \end{pmatrix} - \begin{pmatrix} \lambda_1^2 & & & & \\ \kappa_1^2 & \ddots & & & \\ & \ddots & \lambda_i^2 & & \\ & & \kappa_{i+1}^2 & \lambda_{i+1}^2 & \\ & & & \ddots & \ddots \end{pmatrix} \right] \begin{pmatrix} U_1 \\ \vdots \\ U_i \\ U_{i+1} \\ \vdots \end{pmatrix} =$$

$$\begin{pmatrix} 1 & & & & \\ \Theta & \ddots & & & \\ & \ddots & 1 & & \\ & & \Theta & 1 & \\ & & & \ddots & \ddots \end{pmatrix} \left[p \begin{pmatrix} u_1(0) \\ \vdots \\ u_i(0) \\ u_{i+1}(0) \\ \vdots \end{pmatrix} + \begin{pmatrix} \partial_x u_1|_{x=0} \\ \vdots \\ \partial_x u_i|_{x=0} \\ \partial_x u_{i+1}|_{x=0} \\ \vdots \end{pmatrix} \right]. \quad (7)$$

Denoting the matrix containing the Θ 's by $\mathbf{Q}$ and the matrix containing the λ_j^2 's and κ_j^2 's by $\mathbf{T}$ we write, instead of (7), equivalently

$$(p^2 \mathbf{Q} - \mathbf{T})\{U\} = \mathbf{Q}(p\{u_0\} + \{\partial_x u_0\}). \quad (8)$$

Uniform discretization. Starting with uniform discretization and time-independent exterior potentials, i. e. , $\lambda_1^2 = \lambda_2^2 = \dots = \lambda^2$ and $\kappa_1^2 = \kappa_2^2 = \dots = \kappa^2$, we obtain from (7), using the shift-operator definition,

$$\left(p^2 - \frac{\lambda^2 + s\kappa^2}{1 + s\Theta}\right) \{U\} = p\{u_0\} + \{\partial_x u_0\}. \quad (9)$$

This way, we have expressed the operators $\mathbf{T}$ and $\mathbf{Q}$ completely in terms of the shift operator s . Both $\mathbf{T}$ and $\mathbf{Q}$ are in $\mathcal{C}$, therefore $\mathbf{Q}^{-1}\mathbf{T}$ is in $\mathcal{C}_q$, hence all rational operations with respect to $\mathbf{Q}^{-1}\mathbf{T}$ are well defined. The term $\mathbf{Q}^{-1}\mathbf{T}$ has the algebraic structure of a lower triangular matrix, because $\mathbf{T}$ and $\mathbf{Q}$ are lower triangular matrices. Since $\Im(\lambda^2) \neq 0$, one proves easily that there is always a uniquely defined lower triangular matrix $\mathbf{L}$ such that

$$\mathbf{L} \cdot \mathbf{L} = \mathbf{L}^2 = \mathbf{Q}^{-1}\mathbf{T} \quad \text{with} \quad \Re(\text{diag}(\mathbf{L})) > 0.$$

Formally, we write

$$\mathbf{L} = \sqrt{\frac{\lambda^2 + s\kappa^2}{1 + s\Theta}}. \quad (10)$$

It is clear that for the expression (10) a Taylor series expansion in s at $s = 0$ exists. To any given order, we can take a sufficient number of terms of the series expansion such that the square of the series expansion equals to $\mathbf{Q}^{-1}\mathbf{T}$ up to the given order. Therefore we have equivalently to (10)

$$\mathbf{L} = \lambda + a_1 s + a_2 s^2 + \dots, \quad \text{with} \quad \lambda = \sqrt{\lambda^2}, \Re(\lambda) > 0.$$

Now we obtain the exterior solutions $\{U\}$, as function of the boundary data,

$$\{U\} = \frac{p\{u_0\} + \{\partial_x u_0\}}{(p - \mathbf{L})(p + \mathbf{L})}.$$

The special choice of the boundary conditions

$$\{\partial_x u_0\} = -\mathbf{L}\{u_0\} \quad (11)$$

supplies the desired transparent boundary conditions. This becomes clear, if we consider the related exterior solutions $\{U\}$

$$\{U\} = \frac{\{u_0\}}{p + \mathbf{L}}.$$

Since $\mathbf{L}$ is a lower triangular matrix with real parts of the diagonal entries all greater than zero, it follows that $\{U\}$ contains only decaying modes.

Nonuniform discretization. The difficulty, which appears in generalizing the uniform approach is that the operator $\mathbf{T}$ cannot be expressed in terms of the shift-operator s , because all λ_i^2 's and κ_i^2 's may be different from each other. Nevertheless, the whole approach remains the same, only the simplification of the operator representation is lost. Eq. (8) now reads

$$\left(p^2 + \frac{1}{1 + s\Theta}\mathbf{T}\right)\{U\} = p\{u_0\} + \{\partial_x u_0\}. \quad (12)$$

As the argumentation concerning the factorization of operators $\mathbf{Q}^{-1}\mathbf{T}$ is equally valid here, we solve the problem of the transparent boundary conditions in the nonuniform case, if we find a factorization

$$\mathbf{L} \cdot \mathbf{L} = \mathbf{L}^2 = \frac{1}{1 + s\Theta}\mathbf{T} \quad \text{with} \quad \Re(\text{diag}(L)) > 0.$$

This, however, is a standard task in numerical linear algebra: find the square root of a lower triangular matrix with non-vanishing diagonal elements such that the lower triangular matrix contains only diagonal elements with positive real part. Among these methods are the direct Cholesky-like factorization, which amounts to $\mathcal{O}(i^2)$ operations in the i -th step, Krylov-subspace methods, and suitable basis-transformations, which amount to $\mathcal{O}(i)$ operations. Once $\mathbf{L}$ is obtained, we finally arrive again at the boundary condition (11).

4 Numerical examples

Having outlined the construction of discrete transparent boundary conditions we now investigate the two test cases of [12] associated with optical beam propagation in the Fresnel approximation. The model problems are

$$\begin{aligned} 2in_0k_0\partial_z u &= \partial_x^2 u + (n^2 - n_0^2)k_0^2 u \\ \text{with} \quad k_0 &= 2\pi/\lambda, \quad \lambda = 0.832, \quad n = 1, \end{aligned}$$

with the initial condition and the reference index n_0 in the first case

$$\text{example 1} \quad \begin{cases} u_0(x) = \exp(-(x/10)^2) \exp(-in_0 \sin(\alpha)x) \\ n_0 = \cos(\alpha), \quad \alpha = 21.8^\circ, \end{cases}$$

and in the second case

$$\text{example 2} \quad \begin{cases} u_0(x) = \sum_{j=1,2} \exp(-((x - l_j)/10)^2) \exp(-in_0 \sin(\alpha_j)x) \\ l_1 = -12.5, \quad l_2 = 12.5, \quad \alpha_1 = 26.8^\circ, \quad \alpha_2 = 16.8^\circ \\ n_0 = \cos(\beta), \quad \beta = 21.8^\circ. \end{cases}$$

The first of these involves a single beam with a Gaussian profile propagating in vacuum, $n = 1$, at a wavelength of $0.832\mu\text{m}$ and describing an angle

of $\alpha = 21.8^\circ$ with respect to the z -axis. The computational window has a width of $200\mu m$ and the propagation step length $\Delta z = 0.4\mu m$. The propagation distance of $Z = 500\mu m$ is selected to yield a single reflection from the boundary. The second set of comparisons involves a superposition of two Gaussian beams, one placed at a distance $-12.5\mu m$ from the coordinate origin and propagating at an angle of 26.8° and the second placed at $+12.5\mu m$ from the coordinate origin and propagating at 16.8° . In all test cases a uniform finite-difference discretization in x -direction has been utilized together with the implicit midpoint rule in the direction of propagation (z -axis). In order to visualize the residual reflections the 10^{-10} , 10^{-8} , 10^{-6} , 10^{-4} , 10^{-2} , 10^{-1} iso-lines of $|u(x, z)|^2$, where $u(x, z)$ is the numerically calculated electric field profile normalized with respect to the discrete L^2 -norm such that $\|u(x, 0)\| = 1$, are plotted.

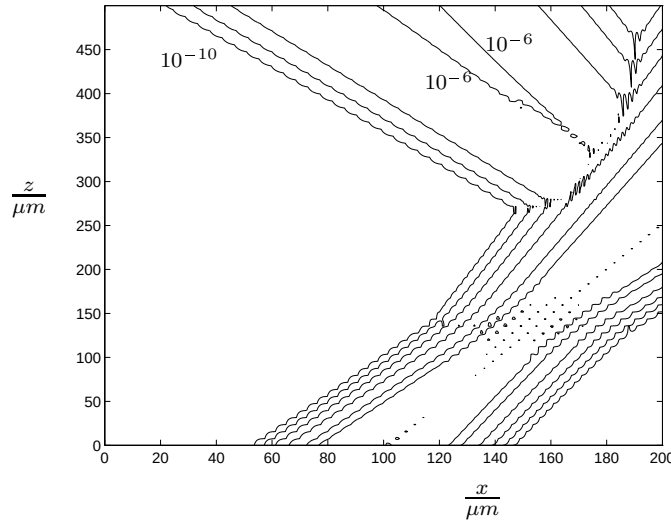


Figure 1: Iso power curves for a two-beam test case with $N = 1024$

Fig. 1 displays the iso-line plot for the test case corresponding to the propagation of a double beam on an uniform $N = 1024$ point transverse grid. The small reflections are produced by the discretization error in the transverse, x , direction.

In order to verify that the magnitude of the reflection depends on the accuracy of the inner solution rather than on the shape of the propagating field, we have repeated our numerical experiments for $N = 8192$ transverse discretization points, generating the results given in Fig. 2. It is evident from this figure that the spurious reflections are suppressed as the accuracy of the inner solution increases.

In Fig. 3, we instead present the discrete L^2 -norm of the field, $u(x, z)$,

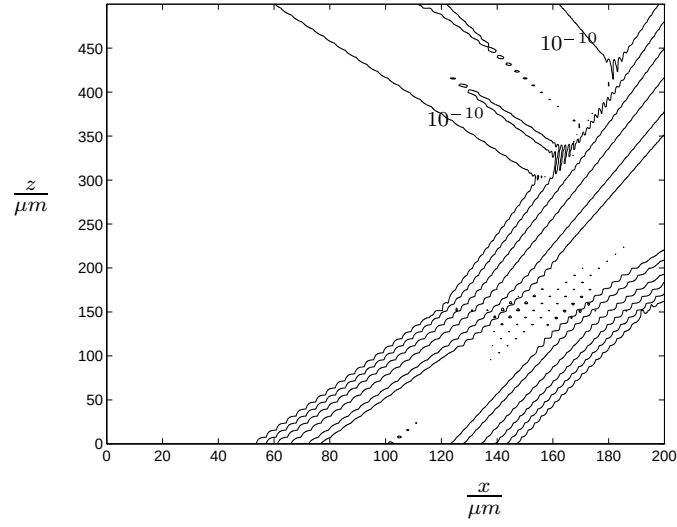


Figure 2: Iso power curves for the two-beam case with $N = 8192$.

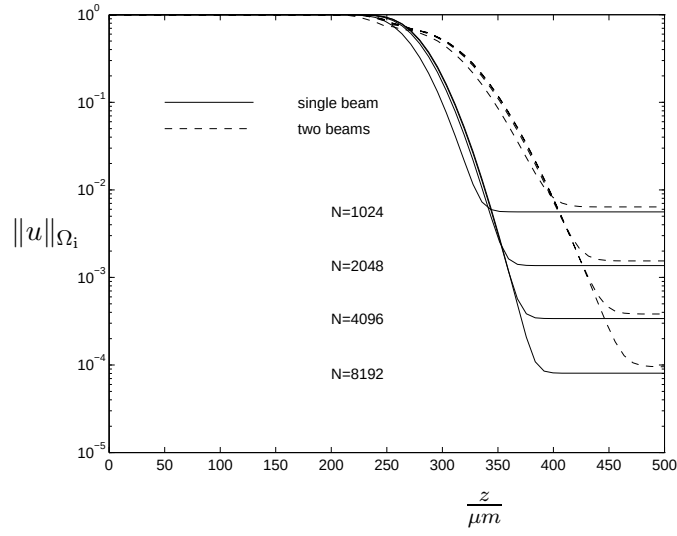


Figure 3: The discrete L^2 -norm of the electric field remaining inside the computational window. The larger the number N of discretization points the smaller becomes the reflected field.

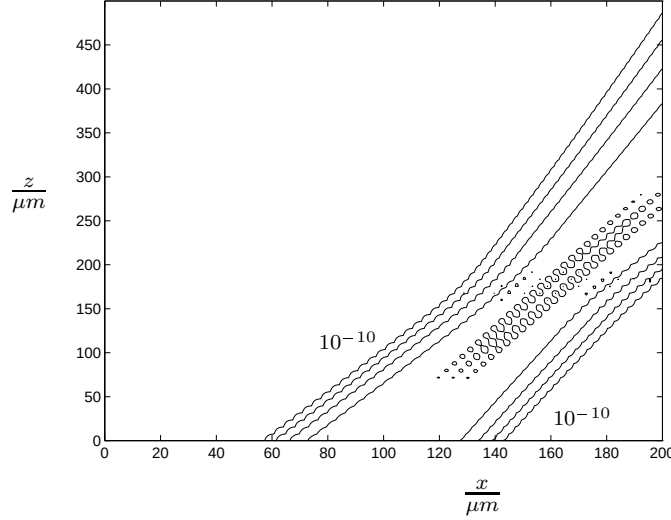


Figure 4: Iso-curves for the two-beam test case with $N = 1024$ in the fully discrete approach

remaining inside the computational window as a function of the number of transverse discretization points. The plateaus in the figures indicate the power reflection coefficient after an integer number of reflections. Clearly, these results confirm that magnitude of the reflection coefficient varies with the x-discretization error of the problem in the interior domain.

Next we demonstrate that the spurious reflections of the previous examples can be avoided with the aid of our fully discrete approach, for uniformly spaced grid points. Repeating our test examples with $N = 1024$ grid points, we thus obtain the iso-lines of Fig. 4 which contain no observable reflected power.

Finally, we discuss the influence of z-dependent exterior refractive indexes, which is equivalent to time dependent exterior potentials in the Schrödinger context. Exactly at the position, where the center of the beam hits the right boundary, the refractive index changes according to

$$n = \begin{cases} 1 & \text{if } z < 250\mu m \\ \frac{1}{2} & \text{if } z \geq 250\mu m \end{cases}.$$

At first, we repeat the double beam experiment with the boundary conditions as before, i. e. , we neglect the occurrence of the refractive index jumps. Of course, for $z \geq 250\mu m$, the boundary conditions become wrong, and a considerable amount of power is reflected (Figs 5 and 6). The factorization of the matrix $(1 + s\Theta)^{-1}\mathbf{T}$, where $\mathbf{T}$ may contain both adaptive step-sizes and index-changes, supplies the desired result (see Fig. 's 7 and 8).

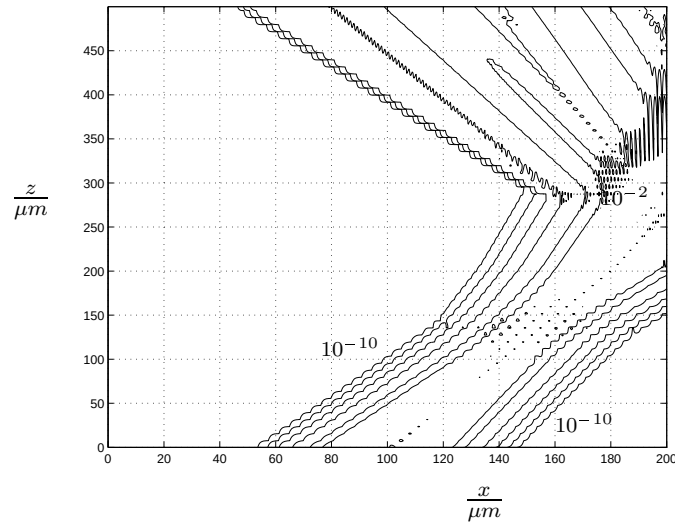


Figure 5: Iso-curves for the two-beam test case with $N = 1024$ and an abrupt index-change at the half of the propagation distance. The boundary conditions are computed with the “uniform” formula, which is wrong in this case (see also Fig. 6)

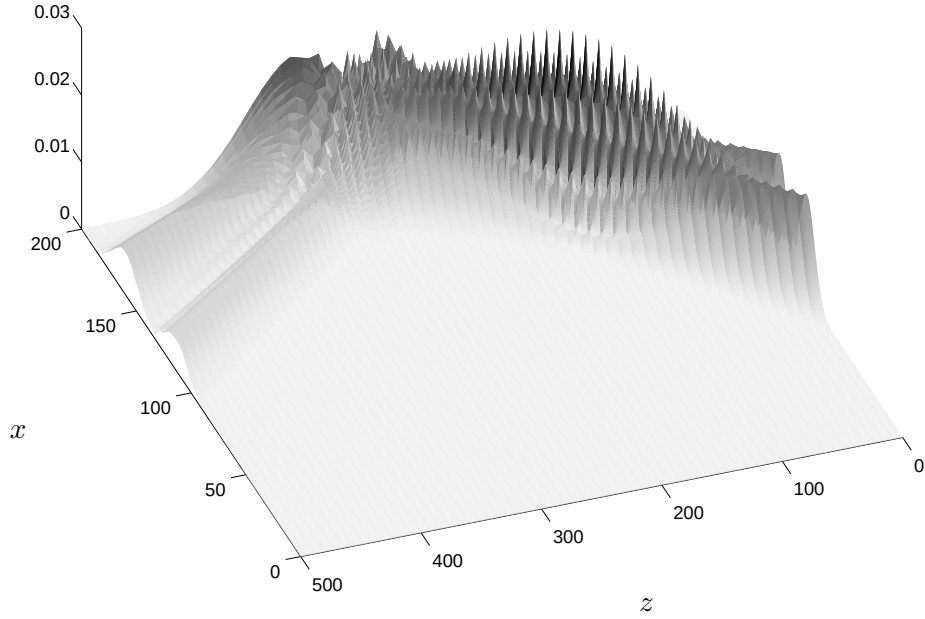


Figure 6: 3D representation of the field evolution for the two-beam test case with abrupt index-change (see also Fig. 5). The computed boundary conditions ignore the index jump.

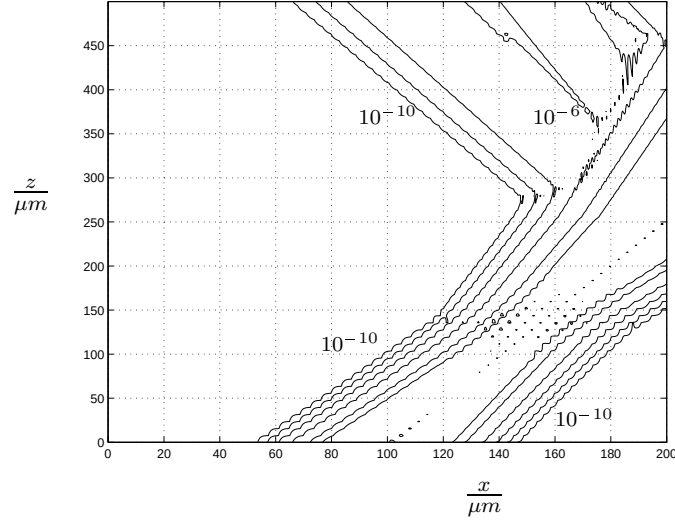


Figure 7: Iso-curves for the two-beam test case with $N = 1024$ and an abrupt index-change at the half of the propagation distance. The boundary conditions take the index-jump into account (see also Fig. 8)

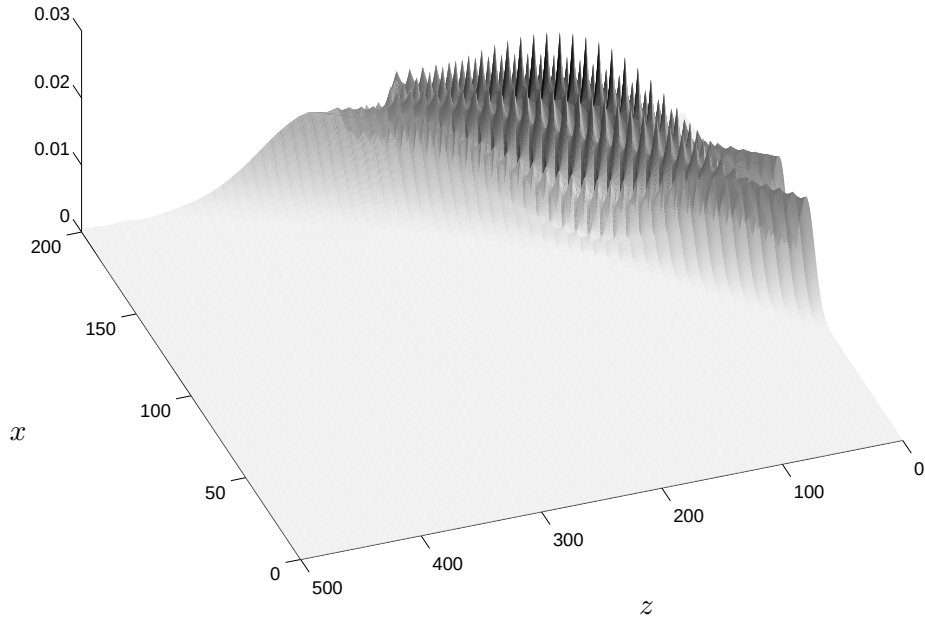


Figure 8: 3D representation of the field evolution for the two-beam test case with abrupt index-change (see also Fig.. 7). The computed boundary conditions take the index-jump into account.

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