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Comparison of the continuous, semi-discrete and fully-discrete Transparent Boundary Conditions (TBC) for the parabolic wave equation 1. Theory

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For the simulation of the propagation of optical waves in open wave guiding structures of integrated optics the parabolic approximation of the scalar wave equation is commonly used. This approach is commonly termed the beam propagation method (BPM). It is of paramount importance to have well-performing transparent boundary conditions applied on the boundaries of the finite computational window, to enable the superfluous portion of the propagating wave to radiate away from the wave guiding structure. Three different formulations (continuous, semi-discrete and fully-discrete) of the non-local transparent boundary conditions are described and compared here.

1. INTRODUCTION

For the computer modelling of the propagation of optical waves in open wave guiding structures of integrated optics often the scalar parabolic wave equation is used. For an accurate solution it is of paramount importance to have appropriate transparent boundary conditions (TBC) formulated on the boundaries of the computational window, which enable the superfluous portion of the propagating wave to radiate away from the computational window and the wave guiding structure, cf. review paper [1].

For the two-dimensional parabolic equation (planar wave guiding structures) usually the continuous transparent boundary condition as formulated by e.g. Baskakov and Popov [2] with its subsequent discretisation has been used for simulations of photonic structures [3]. However, by the *ad hoc* discretisation of the continuous formulae an extra error is introduced. The semi-discrete formulations either in transversal or in the longitudinal variable [4], [9], [10] may improve the situation.

Recently published fully-discrete formulation of the transparent boundary conditions [5] is naturally compatible with the fully discrete finite-differences Crank-Nicolson method of solving the parabolic wave equation. This solution method is nowadays commonly termed the beam propagation method (BPM), although originally the BPM had a special meaning for splitting the parabolic equation into two equations, first representing the free-space diffraction and the second representing the focusation of the wave by a phase screen.

In the case of longitudinally invariant planar structures the propagation of the electromagnetic waves in scalar and parabolic approximation is governed by the Maxwell equations

$$\mathrm{curl}\,\boldsymbol{E}(\boldsymbol{r},t) = -\mu\frac{\partial \boldsymbol{H}(\boldsymbol{r},t)}{\partial t}, \qquad \mathrm{curl}\,\boldsymbol{H}(\boldsymbol{r},t) = \varepsilon\frac{\partial \boldsymbol{E}(\boldsymbol{r},t)}{\partial t}, \tag{1}$$

where the electromagnetic field vectors and material constants have their usual meaning. By a usual procedure from (1) the wave equation

$$\nabla^2 f(\boldsymbol{r},t) - \mu\varepsilon\frac{\partial^2 f(\boldsymbol{r},t)}{\partial t^2} = 0 \tag{2}$$

for any Cartesian component $f(\boldsymbol{r},t)$ of the field vectors $\boldsymbol{E}(\boldsymbol{r},t)$, $\boldsymbol{H}(\boldsymbol{r},t)$ can be obtained. For a monochromatic, i.e. harmonically-in-time oscillating, wave in the complex representation given by

$$f(\boldsymbol{r},t)=\varphi(\boldsymbol{r})\exp(\mathrm{j}\omega t) \quad (3)$$

one obtains for the complex wave amplitude $\varphi(\boldsymbol{r})$ the equation

$$\nabla^2\varphi(\boldsymbol{r})+\beta^2\varphi(\boldsymbol{r})=0\,, \quad (4)$$

where $\beta=\omega\sqrt{\mu\varepsilon}$ is the propagation coefficient.

If the wave has a dominant direction of propagation, say y in Cartesian coordinates, then one can strip-off rapid oscillations in this direction from the complex wave amplitude by the slowly-varying-envelope substitution

$$\varphi(x,y,z)=\psi(x,y,z)\exp(-\mathrm{j}ky)\,, \quad (5)$$

where usually $k\approx\beta$. Then instead of (4) one obtains for $\psi(\boldsymbol{r})$ the equation

$$-2\mathrm{j}k\frac{\partial\psi}{\partial y}+\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}+\left[\beta^2-k^2\right]\psi=0\,.(6)$$

For the wave propagation in homogeneous space, where $\mu,\varepsilon=const$, k can be set equal to β and (6) simplifies into

$$-2\mathrm{j}k\frac{\partial\psi}{\partial y}+\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}=0\,. \quad (7)$$

In what follows we shall consider only two-dimensional problems (planar structures), i.e. the spatial coordinate variable z is omitted. If the spatial variations of the amplitude envelope ψ are slow compared to the fast oscillations of the carrier frequency, i.e. $\partial\psi/\partial y << k$, then the second derivative with respect to y in (7) can be neglected and one arrives to the wave equation in parabolic approximation (sometimes called the Fresnel equation)

$$-2\mathrm{j}k\frac{\partial\psi}{\partial y}+\frac{\partial^2\psi}{\partial x^2}+\left[\beta^2-k^2\right]\psi=0\,. \quad (8)$$

Here the variable x means the "transversal" coordinate and the wave dominantly propagates along the "longitudinal" coordinate y.

The simplest solution to (4) is the homogeneous plane wave propagating in e.g. y-direction

$$\varphi(\boldsymbol{r})=A\exp(-\mathrm{j}\beta y)\,, \quad (9)$$

where A is a constant and $\lambda=2\pi/\beta$ is the wavelength of the plane wave.

Any wave amplitude can be expanded into the spectrum of obliquely propagating plane waves. In two dimensions for the obliquely propagating homogeneous plane wave one obtains instead of (9) the formula

$$\varphi(\boldsymbol{r})=A\exp(-\mathrm{j}q_x x)\exp(-\mathrm{j}q_y y)\,, \quad (10)$$

where q_x and q_y are transversal and longitudinal wavenumbers (spatial frequencies). The wave equation (4) yields the "dispersion relation"

$$q_y=\sqrt{\beta^2-q_x^2} \quad (11)$$

imposing thus an upper limit on transversal spatial frequencies $q_x\le\beta$. Beyond this limit only evanescent plane waves exist.

For the slowly-varying-envelope formulation (5) one can instead of (10)write

$$\psi(\boldsymbol{r})=A\exp(-\mathrm{j}q_x x)\exp(-\mathrm{j}q_y y)\exp(\mathrm{j}ky)=$$

$$=A\exp(-\mathrm{j}q_x x)\exp(-\mathrm{j}\kappa y)\,. \quad (12)$$

For the pertaining exact equation (6) the same dispersion relation (11) holds. However, the parabolic approximation (8) yields for (12) the dispersion relation

$$\kappa=q_y-k=(\beta^2-k^2-q_x^2)/2k\approx-q_x^2/2k \quad (13)$$

without any upper limit on q_x. The wave amplitude envelope $\psi(\boldsymbol{r})$ possesses indeed only slow longitudinal variations characterised by the spatial frequency - the wavenumber $\kappa\ll q_x$.

In the case of the wave guiding structures the propagation coefficient β may be a function of the transversal variable $\beta=\beta(x)$ on some finite domain. Particularly for homogeneous waveguides it is a kind of piecewise-constant function.

2. CONTINUOUS TRANSPARENT BOUNDARY CONDITIONS

If the equation (8) should be solved numerically the transversal variable x must be bounded to some interval, say $x\in(0,x_{\max})$ called computational window. In course of wave propagation the wave front changes due to the self-diffraction, the wave, in general, diverges (apart of some special cases) and thus also the wavefront originally bounded within the computational window reaches the boundaries and will be out-radiated throughout the computational window.

The problem of transparent boundaries consists in formulating such boundary conditions for $\psi(x,y)$ that on the "left" boundary $x=0$ only the wave propagating to the left, and on the "right" boundary $x=x_{\max}$ only the wave propagating to the right exists, i.e. no reflections on the boundaries occur. The parabolic wave equation (8) can be formally written as

$$\left\{\frac{\partial}{\partial x}-\mathrm{j}\sqrt{\left[\beta^2-k^2\right]-2\mathrm{j}k\frac{\partial}{\partial y}}\right\}\times$$

$$\times\left\{\frac{\partial}{\partial x}+\mathrm{j}\sqrt{\left[\beta^2-k^2\right]-2\mathrm{j}k\frac{\partial}{\partial y}}\right\}\psi=0 \quad (14)$$

and further factorised into two "one-way" equations, i.e.

$$\left\{\frac{\partial}{\partial x}-\mathrm{j}\sqrt{\left[\beta^2-k^2\right]-2\mathrm{j}k\frac{\partial}{\partial y}}\right\}\psi=0, \quad (15)$$

and

$$\left\{\frac{\partial}{\partial x}+\mathrm{j}\sqrt{\left[\beta^2-k^2\right]-2\mathrm{j}k\frac{\partial}{\partial y}}\right\}\psi=0, \quad (16)$$

yielding thus the formal solution

$$\psi(x,y)=$$

$$=\exp\left\{\pm\mathrm{j}(x-x_0)\sqrt{\left[\beta^2-k^2\right]-2\mathrm{j}k\frac{\partial}{\partial y}}\right\}\times$$

$$\times\psi(x_0,y), \quad (17)$$

where the plus or minus sign in (17) denotes the wave propagating either "to the left" or "to the right" with respect to the x axis,

The transparent boundary conditions have to guarantee that the wave amplitude fulfils on the left boundary $x=0$ relation (17) with the upper sign and on the right boundary $x=x_{\max}$ with the lower sign.

Taking the Laplace transform of $\psi(x,y)$ in y-variable, i.e.

$$\Psi(x,p)=\int_0^{\infty}\psi(x,y)\exp(-py)dy, \quad (18)$$

and substituting it into the parabolic wave equation (8) yields

$$-2\mathrm{j}kp\Psi(x,p)+\frac{\partial^2\Psi(x,p)}{\partial x^2}+$$

$$+\left[\beta^2-k^2\right]\Psi(x,p)=0. \quad (19)$$

Solution of (19) for $x\le 0$, or $x\ge x_{\max}$, reads

$$\Psi_{1,2}(x,p)=$$

$$=\Psi(x_0,p)\exp\left\{\pm\mathrm{j}(x-x_0)\sqrt{\beta^2-k^2-2\mathrm{j}kp}\right\}, \quad (20)$$

where always the branch of the square root with positive real part is taken. Thus (20) represents two transversally propagating waves, either along the negative (upper sign) or along the positive (lower sign) direction of the *x*-axis. These two solutions represent in the Laplace transform domain the solution (17) of the two corresponding "one-way" wave equations (16).

Differentiating (20) yields the relation between $\Psi(x,p)$ and its derivative $\partial\Psi(x,p)/\partial x$

$$\frac{\partial\Psi(x,p)}{\partial x}=\sqrt{A(p)}\Psi(x,p), \quad (21)$$

where

$$A(p)=2\mathrm{j}kp-(\beta^2-k^2), \quad (22)$$

or in the so called impedance form

$$\Psi(x,p)=\frac{1}{\sqrt{A(p)}}\frac{\partial\Psi(x,p)}{\partial x}. \quad (23)$$

The inverse Laplace transform $f(y)$ of the weighting function $F(p)$ in (23),

$$F(p)=1/\sqrt{A(p)}=1/\sqrt{2\mathrm{j}kp-(\beta^2-k^2)}, \quad (24)$$

can be, by using the Laplace transform pair

$$1/\sqrt{p}\Leftrightarrow 1/\sqrt{\pi y}, \quad (25)$$

together with the properties of the Laplace transform

$$\begin{aligned}F(\alpha p)&\Leftrightarrow\alpha^{-1}f(y/\alpha)\\ F(p-a)&\Leftrightarrow f(y)\exp(-ay)\end{aligned}, \quad (26)$$

easily obtained in the form

$$f(y)=\frac{1}{\sqrt{2\mathrm{j}k\pi y}}\exp\left(-\mathrm{j}\frac{\beta^2-k^2}{2k}y\right), \quad (27)$$

or for the case $k=\beta$ in the simpler form

$$f(y)=\frac{1}{\sqrt{2\mathrm{j}k\pi y}}. \quad (28)$$

The inverse Laplace transform of (23) is then expressed as the convolution integral

$$\psi(x,y)=\frac{\partial\psi(x,y)}{\partial x}\otimes f(y)=$$

$$=\int_0^y\frac{\partial\psi(x,\zeta)}{\partial x}f(y-\zeta)d\zeta \quad (29)$$

i.e. it yields the convolution integral

$$\psi(x,y)=\frac{1}{\sqrt{2\mathrm{j}\pi k}}\int_0^y\frac{1}{\sqrt{y-\zeta}}\times$$

$$\times \exp\left[-\mathrm{j}\frac{\beta^2-k^2}{2k}(y-\zeta)\right]\frac{\partial\psi(x,\zeta)}{\partial x}d\zeta \quad (30)$$

For $k=\beta$ one obtains the simplified result

$$\psi(x,y)=\frac{1}{\sqrt{2\mathrm{j}\pi k}}\int_0^y \frac{1}{\sqrt{y-\zeta}}\frac{\partial\psi(x,\zeta)}{\partial x}d\zeta \quad (31)$$

identical with the original Baskakov & Popov's formula [1].

In (30) and (31) the values in the boundary points $(x,y)=(0,y_0)$, or $(x,y)=(x_{\max},y_0)$ are expressed through the derivative of the boundary values in all "previous" boundary points, e.g. in the boundary point $x=0$ all values $\partial\psi(x,y)/\partial x|_{x=0}$ for $y\in(0,y_0)$ play the role in (30) and (31). Similar holds in the boundary point $x=x_{\max}$ too.

Thus both formulas (30) and (31) are non-local with respect to the propagation coordinate y, i.e. with growing upper bound of the convolution integral (31) the integration path increases too, requiring more computational resources, which in fact rather complicates their application.

To prevent the growth of the length of the integration interval with growing y_0, at least within certain accuracy, "the cut-off strategy" can be applied. After an initial integration phase with integration interval $(0,y_0)$, $y_0\le\Theta$, for $y_0>\Theta$ the "sliding integration interval"approach is taken i.e. the length of the integration interval in (30) and (31) remains constant and equals $(y_0-\Theta,y_0)$ instead of $y\in(0,y_0)$.

Thus, using (30), or (31) the reflections of waves in the boundary points $x=0$ and $x=x_{\max}$ can be prohibited.

3. SEMI-DISCRETE APPROACH I: THE DISCRETISED TRANSVERSAL DIRECTION

For the numerical simulations using digital computers the wave-amplitude profile $\psi(x,y)$ has to be calculated on the discrete mesh, i.e. the values $\psi(x,y)$ are to be taken on the set of discrete points (x_m,y_n)

$$\psi(x_m,y_n)=\psi(m\Delta_x,n\Delta_y) \quad (32)$$

for $m=0,1,2,...,M$, where Δ_x and Δ_y are equidistant discretisation intervals. The computational window is selected to be $(0,x_{\max})=(0,M\Delta_x)$. The index $n=0,1,2,...,$ denotes subsequent layers of wave-amplitude values in the propagation direction.

Let us first consider the discretisation along the transversal coordinate x only, taking the values $\psi_m(y)$ in equidistant grid points $x_m=m\Delta_x$, i.e.

$$\psi(x_m,y)=\psi(m\Delta_x,y)=\psi_m(y). \quad (33)$$

The second derivative in (8) is replaced by the second central difference quotient

$$\frac{\partial^2\psi(x,y)}{\partial x^2}\approx\frac{\psi_{m+1}(y)-2\psi_m(y)+\psi_{m-1}(y)}{\Delta_x^2} \quad (34)$$

and instead of (8) one obtains the approximation in form of the finite difference equation

$$-2\mathrm{j}k\frac{\partial\psi_m(y)}{\partial y}+\frac{\psi_{m+1}(y)-2\psi_m(y)+\psi_{m-1}(y)}{\Delta_x^2}+$$

$$+\left[\beta^2-k^2\right]\psi_m(y)=0. \quad (35)$$

Now the same strategy as in (19) can be used and after applying the Laplace transform with respect to y it yields

$$\frac{\Psi_{m+1}(p)-2\Psi_m(p)+\Psi_{m-1}(p)}{\Delta_x^2}+$$

$$+\left[\beta^2-k^2-2\mathrm{j}kp\right]\Psi_m(p)=0. \quad (36)$$

The solution of the ordinary finite difference equation of the second order (36) reads

$$\Psi_m(p)=\frac{\Psi_{m+1}(p)}{1+B(p)+\sqrt{2B(p)+B^2(p)}}, \quad (37)$$

or in the impedance form

$$\Psi_m(p)=\frac{\Psi_{m+1}(p)-\Psi_m(p)}{B(p)+\sqrt{2B(p)+B^2(p)}}, \quad (38)$$

where we have introduced the abbreviation

$$B(p)=\frac{\Delta_x^2}{2}A(p)=\frac{\Delta_x^2}{2}\left\{2\mathrm{j}kp-(\beta^2-k^2)\right\}. \quad (39)$$

Both weighting functions in (37) and (38)

$$H(p)=\frac{1}{1+B(p)+\sqrt{2B(p)+B^2(p)}}, \quad (40)$$

$$G(p)=\frac{1}{B(p)+\sqrt{2B(p)+B^2(p)}} \quad (41)$$

can be exactly inverted using the Laplace transform properties (26) and the Laplace transform pairs

$$\left\{1+p+\sqrt{2p+p^2}\right\}^{-1}\Leftrightarrow y^{-1}\exp(-y)I_1(y), \quad (42)$$

$$\left\{p+\sqrt{2p+p^2}\right\}^{-1} \Leftrightarrow \tfrac{1}{2}\exp(-y)\left[I_0(y)+I_1(y)\right], \quad (43)$$

where $I_0(y)$ and $I_1(y)$ are modified Bessel functions, yielding thus the results in the convolution form

$$\psi_m(y) = \int_0^y \psi_{m+1}(\zeta) h(y-\zeta) d\zeta , \quad (44)$$

$$\psi_m(y) = \int_0^y \left[\psi_{m+1}(\zeta) - \psi_m(\zeta)\right] g(y-\zeta) d\zeta . \quad (45)$$

Use of asymptotic expressions for large y in the Bessel functions yields for (43) the formula

$$\tfrac{1}{2}\exp(-y)\left[I_0(y)+I_1(y)\right] \approx 1/\sqrt{2\pi y}, \; y \gg 1 . \quad (46)$$

Thus $g(y) \approx f(y)/\Delta_x$ for $y \gg k\Delta_x^2$, where $f(y)$ is given by (27). On the other hand for $y \ll k\Delta_x^2$ the behaviour of the kernel function $g(y)$ is completely different from $f(y)$ as seen from (43) for the limiting case of small y, i.e.

$$\tfrac{1}{2}e^{-y}\left[I_0(y)+I_1(y)\right] \approx \tfrac{1}{2} - \tfrac{1}{4}y + \tfrac{1}{8}y^2, \; y \ll 1 . \quad (47)$$

Apparently, the main difference between convolution-kernel-functions $f(y)$ in (29) for continuous TBC and $g(y)$ in (45) for semi-discrete TBC formulation occurs for small arguments, i.e. in the vicinity of the point y, when $\zeta \sim y$, where the TBC is going to be determined.

The weighting function $G(p)$ in (41) can be written also as the product

$$G(p) = \frac{1}{\sqrt{2B(p)}}\left\{\sqrt{1+B(p)/2} - \sqrt{B(p)/2}\right\} . \quad (48)$$

Here the Laplace transform pair of the first factor

$$1/\sqrt{2B(p)} \Leftrightarrow f(y)/\Delta_x \quad (49)$$

corresponds in fact to the kernel function $f(y)$ pertaining to the continuous TBC accordingly to (27), or (28), and the second factor in (48)

$$D(p) = \sqrt{1+B(p)/2} - \sqrt{B(p)/2} \quad (50)$$

yields using the Laplace transform pair

$$\frac{1}{\sqrt{1+p/2}+\sqrt{p/2}} \Leftrightarrow \frac{1-e^{-2y}}{2y\sqrt{2\pi y}} , \quad (51)$$

the kernel function

$$d(y) = \Delta_x\sqrt{jk}\,\frac{1-\exp\left(-2y/jk\Delta_x^2\right)}{2y\sqrt{2\pi y}} \quad (52)$$

This result can be interpreted in terms of the double convolution

$$\phi_m(y) = \int_0^y \frac{\psi_{m+1}(\zeta)-\psi_m(\zeta)}{\Delta_x} f(y-\zeta) d\zeta \quad (53)$$

$$\psi_m(y) = \int_0^y \phi_m(\zeta) d(y-\zeta) d\zeta \quad (54)$$

The first convolution (53) yields an intermediate result $\phi_m(y)$ and it is in fact the same formula as (29) for the continuous TBC when one substitutes the first difference quotient $(\psi_{m+1}-\psi_m)/\Delta_x$ in the place of the first derivative $\partial\psi/\partial x$ in (29). The second convolution formula (54) illustrates the effect of the semi-discrete formulation of the TBC in comparison with the continuous TBC in terms of the second convolution with the kernel function $d(y)$.

For $\Delta_x \to 0$ the kernel function $d(y)$ converges to the delta function, $d(y) \to \delta(y)$ as can be easily seen in the Laplace-transform domain since $D(p) \to 1$ for $\Delta_x \to 0$. Then $\psi_m(y) = \phi_m(y)$ and (53) is identical with (29). Herewith the link to the continuous TBC is completely established.

For the small values of y, $y \ll k\Delta_x^2$ one obtains asymptotically

$$d(y) \approx \frac{1}{\Delta_x\sqrt{2jk\pi y}} , \quad (55)$$

while for large y, $y \gg k\Delta_x^2$,

$$d(y) \approx \frac{\Delta_x\sqrt{jk}}{2y\sqrt{2\pi y}} \quad (56)$$

holds, and both together confirm the delta-function-like behaviour of $d(y)$ for $\Delta_x \to 0$.

4. SEMI-DISCRETE APPROACH II: THE DISCRETISED PROPAGATION DIRECTION

Instead of discretising $\psi(x,y)$ along the transversal direction x as in (35), alternatively the discretisation along the longitudinal direction y can be taken, i.e. one takes the values $\psi_n(x)$ in equidistant points $y_n = n\Delta_y$, $n = 0, 1, 2, ...$ where

$$\psi(x, y_n) = \psi(x, n\Delta_y) = \psi_n(x) \quad (57)$$

Using the explicit-implicit Crank-Nicolson strategy (trapezoidal rule) the semi-discretised formulation of (8) takes the form

$$-4\mathrm{j}k\frac{\psi_{n+1}(x)-\psi_n(x)}{\Delta_y}+\left[\frac{\partial^2\psi_{n+1}(x)}{\partial x^2}+\frac{\partial^2\psi_n(x)}{\partial x^2}\right]+$$

$$+\left[\beta^2-k^2\right]\left[\psi_{n+1}(x)+\psi_n(x)\right]=0, \quad (58)$$

where the first derivative with respect to y was replaced by the central first difference quotient with the step size $\Delta_y/2$ and the function value itself by the average of values in the forward and backward half-step

$$\frac{\partial\psi_{n+1/2}(x)}{\partial y}\approx\frac{\psi_{n+1}(x)-\psi_n(x)}{\Delta_y},$$
$$\psi_{n+1/2}(x)\approx\frac{\psi_{n+1}(x)+\psi_n(x)}{2}, \quad (59)$$

Instead of the Laplace transform as in (18) for continuous $\psi(x,y)$ it is now quite natural to take the *Z*-transform (see Appendix 1)

$$\Psi(x,z)=\sum_{n=0}^{\infty}\psi_n(x)z^{-n} \quad (60)$$

for the discrete sequence $\{\psi_n(x)\}_{n=0,1,2,..}$.

Using the "shift" property (149) in Appendix 1 of the *Z*-transform (58) yields

$$\frac{\partial^2\Psi(x,z)}{\partial x^2}+$$
$$+\left\{\left[\beta^2-k^2\right]-\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}\right\}\Psi(x,z)=0, \quad (61)$$

with the solution analogous to (20)

$$\Psi_{1,2}(x,z)=\Psi(x_0,z)\times$$
$$\times\exp\left\{\pm\mathrm{j}(x-x_0)\sqrt{\beta^2-k^2-\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}}\right\}. \quad (62)$$

In analogy to (21) one obtains another kind of the semi-discrete transparent boundary condition

$$\frac{\partial\Psi(x,z)}{\partial x}=\sqrt{A(z)}\Psi(x,z), \quad (63)$$

where

$$A(z)=\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}-(\beta^2-k^2). \quad (64)$$

In the impedance form it reads

$$\Psi(x,z)=\frac{1}{\sqrt{A(z)}}\frac{\partial\Psi(x,z)}{\partial x}. \quad (65)$$

Note that $A(z)$ equals $A(p)$ in (22) for

$$p=\frac{2}{\Delta_y}\frac{z-1}{z+1}. \quad (66)$$

In the "homogeneous space" case, i.e. if $k=\beta$, (64) is simplified into

$$A(z)=\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}. \quad (67)$$

Then (63), or (65) can be easily inverted using (144) in Appendix 1. The resulting discrete convolution formulae then are

$$\frac{\partial\psi_N(x)}{\partial x}=\sqrt{\frac{4\mathrm{j}k}{\Delta_y}}\sum_{n=0}^{N}b_n\psi_{N-n}(x), \quad (68)$$

or

$$\psi_N(x)=\sqrt{\frac{\Delta_y}{4\mathrm{j}k}}\sum_{n=0}^{N}a_n\frac{\partial\psi_{N-n}(x)}{\partial x}, \quad (69)$$

with the sequences (144)

$$\left.\begin{Bmatrix}a_n\\b_n\end{Bmatrix}\right|_{n=0,1,2,..}=\left\{1,\pm1,\frac{1}{2},\pm\frac{1}{2},\frac{1\cdot3}{2\cdot4},\right.$$
$$\left.\pm\frac{1\cdot3}{2\cdot4},\frac{1\cdot3\cdot5}{2\cdot4\cdot6},\pm\frac{1\cdot3\cdot5}{2\cdot4\cdot6},....\right\}, \quad (70)$$

where for $\{a_n\}$ the upper signs and for $\{b_n\}$ the lower ones apply.

It should be noticed, that using the *Z*-transform instead of the Laplace transform, a significant advantage of having, in the case $k\neq\beta$, in convolution formulas of the type (30) the simple multiplicative factors

$$\exp\left[-\mathrm{j}\frac{\beta^2-k^2}{2k}(y-\zeta)\right], \quad (71)$$

is lost.

The link between the continuous solution formulated in (21) and (22) in form of the Laplace transform and the semi-discrete solution formulated in (63) and (64) can be easily established. As it is well known if one represents a discrete sequence $\{f_n\}_{n=0,1,2,..}$ by the stair-case function

$$f(y)=$$
$$=\sum_{n=0}^{\infty}f_n\left\{U(y-n\Delta_y)-U(y-n\Delta_y-\Delta_y)\right\}, \quad (72)$$

where $U(y)$ is the unit-step function, then the Laplace transform of $f(y)$ equals

$$F(p) = \frac{1-\exp(p\Delta_y)}{p} \sum_{n=0}^{\infty} f_n \exp(-np\Delta_y) \text{ ,(73)}$$

where the summation term is equal to the Z-transform (137) with the argument $z = \exp(p\Delta_y)$. Then from (64) one obtains

$$A(p) = \frac{4\,\mathrm{j}k}{\Delta_y} \frac{\exp(p\Delta_y)-1}{\exp(p\Delta_y)+1} - (\beta^2 - k^2), \quad (74)$$

which in form of (21) represents the solution of the difference equation (58) in terms of the Laplace transform of a stair-case function (72). In the limiting case of negligible Δ_y, $\Delta_y \to 0$, one obtains the result

$$A(p) \approx 2\,\mathrm{j}k\left(p + p^2\Delta_y^2/2 + \ldots\right) - (\beta^2 - k^2) \text{ ,(75)}$$

being in the first approximation identical with (22).

5. NUMERICAL IMPLEMENTATION OF THE COUNTINUOUS TRANSPARENT BOUNDARY CONDITIONS.

The numerical approximation to (31) is obtained by the same discretisation of the propagation path variable y into the equidistant intervals as in (57). The discretised form of the continuous convolution formula (31) then reads, either by using the trapezoidal rule

$$\psi_N(x) = \frac{1}{\sqrt{2\mathrm{j}\pi k}} \sum_{n=1}^{N} \frac{1}{2}\left[\frac{\partial\psi_{n-1}(x)}{\partial x} + \frac{\partial\psi_n(x)}{\partial x}\right] \times$$

$$\times \int_{y_{n-1}}^{y_n} \frac{1}{\sqrt{y_N - \zeta}} d\zeta, \quad (76)$$

or by using the linear interpolation

$$\psi_N(x) = \frac{1}{\sqrt{2\mathrm{j}\pi k}} \sum_{n=1}^{N} \int_{y_{n-1}}^{y_n} \frac{1}{\sqrt{y_N - \zeta}} \times$$

$$\times \left[\frac{\partial\psi_{n-1}(x)}{\partial x}\frac{y_n - \zeta}{\Delta_y} + \frac{\partial\psi_n(x)}{\partial x}\frac{\zeta - y_{n-1}}{\Delta_y}\right] d\zeta. \quad (77)$$

After having integrated (76), or (77) respectively, one obtains again a formula of the type (69). The integration in (76) and in (77) can be easily performed and yields

$$\{a_n\} = \begin{cases} \sqrt{\frac{2}{\pi}}, n = 0 \\ \left\{\sqrt{\frac{2}{\pi}}\left[\sqrt{n+1} - \sqrt{n-1}\right]\right\} \\ \sqrt{\frac{2}{\pi}}\left[\sqrt{N} - \sqrt{N-1}\right], n = N \end{cases} \quad (78)$$

for (76) and

$$\{a_n\} = \begin{cases} \frac{4}{3}\sqrt{\frac{2}{\pi}}, n = 0 \\ \left\{\frac{4}{3}\sqrt{\frac{2}{\pi}}\left[(n+1)^{3/2} + (n-1)^{3/2} - 2n^{3/2}\right]\right\} \\ \frac{4}{3}\sqrt{\frac{2}{\pi}}\left[(N-1)^{3/2} - N^{3/2} + 6\sqrt{N}\right], n = N \end{cases} \quad (79)$$

for (77).

When (78) or (79) is used to calculate $\{a_n\}$ then the problem of “subtractive cancellation” occurs, i.e. there are rounding-error-problems with subtraction of two slightly differing large numbers due to their representation in the digital computer by a finite number of digits. Therefore one can better use the transformed formulas, i.e.

$$\{a_n\} = \begin{cases} \sqrt{\frac{2}{\pi}}, n = 0 \\ \left\{\sqrt{\frac{2}{\pi}}\left[2/\left(\sqrt{n+1} + \sqrt{n-1}\right)\right]\right\} \\ \sqrt{\frac{2}{\pi}}\left[1/\left(\sqrt{N} + \sqrt{N-1}\right)\right], n = N \end{cases} \quad (80)$$

for (78), and

$$\{a_n\} =$$

$$= \begin{cases} \frac{4}{3}\sqrt{\frac{2}{\pi}}, n = 0 \\ \left\{\frac{4}{3}\sqrt{\frac{2}{\pi}}\left[\frac{3n^2+3n+1}{(n+1)^{3/2}+n^{3/2}} - \frac{3n^2-3n+1}{(n-1)^{3/2}+n^{3/2}}\right]\right\} \\ \frac{4}{3}\sqrt{\frac{2}{\pi}}\left[6\sqrt{N} - \frac{3N^2-3N+1}{(N-1)^{3/2}+N^{3/2}}\right], n = N \end{cases} (81)$$

for (79). The “subtractive cancellation” problem persists in (81) too, but is of lower order than in (79).

Numerical values for $\{a_n\}$ accordingly the three different formulations(70), (78) and (79) are shown in Table 1 and Table 2. It can be seen that the coefficients $\{a_n\}$ are substantially different between individual columns only for small n. The coefficients in the first column are paired with the same value while in the last two columns they are symmetrically distributed with respect to the values in the first column. This confirms numerically the asymptotic equivalence of continuous and semi-discrete approach. Nevertheless, whatever small the discretisation interval Δ_y is, the different sequences $\{a_n\}$ pertaining to the particular method of the three discretisations remain.

Table 1. Values of $\{a_n\}$ accordingly the respective formula

n	**Formula** (70)	**Formula** (78)	**Formula** (79)
0	1.000000	0.797885	1.063846
1	1.000000	1.128379	0.881319
2	0.500000	0.584092	0.573730
3	0.500000	0.467390	0.463967
4	0.375000	0.402148	0.400530
5	0.375000	0.358641	0.357727
6	0.312500	0.326880	0.326305
7	0.312500	0.302348	0.301959
8	0.273438	0.282650	0.282372
9	0.273438	0.266374	0.266167

Table 2. Values of $\{a_n\}$ accordingly the respective formula

n	**Formula** (70)	**Formula** (78)	**Formula** (79)
20	0.176197	0.178468	0.178440
21	0.176197	0.174162	0.174137
30	0.144464	0.145693	0.145683
31	0.144464	0.143323	0.143314
40	0.125371	0.126166	0.126162
41	0.125371	0.124618	0.124613
50	0.112275	0.112844	0.112841
51	0.112275	0.111732	0.111729

6. FULLY-DISCRETE METHOD: DISCRETISED TRANSVERSAL AND PROPAGATION DIRECTIONS

Taking the two-dimensional array of discrete values

$$\psi(x_m, y_n) = \psi(m\Delta_x, n\Delta_y) = \psi_m^n \qquad (82)$$

and using the central second difference quotients in the Crank-Nicolson discretisation scheme one arrives to the discrete formula analogous to (58)

$$-4\mathrm{j}k\frac{\psi_m^{n+1}-\psi_m^n}{\Delta_y}+$$

$$+\left[\frac{\psi_{m+1}^{n+1}-2\psi_m^{n+1}+\psi_{m-1}^{n+1}}{\Delta_x^2}+\frac{\psi_{m+1}^{n}-2\psi_m^{n}+\psi_{m-1}^{n}}{\Delta_x^2}\right]+$$

$$+\left[\beta^2-k^2\right]\left[\psi_m^{n+1}+\psi_m^n\right]=0. \qquad (83)$$

This Crank-Nicolson formula is known to conserve the power of the wave within the infinite computational window and therefore it is especially suitable for wave propagation computations.

Again after having (83) Z-transformed in the propagation-direction variable y one obtains the fully discrete pendant to (61)

$$\frac{\Psi_{m+1}(z)-2\Psi_m(z)+\Psi_{m-1}(z)}{\Delta_x^2}+$$

$$+\left\{\left[\beta^2-k^2\right]-\frac{4\mathrm{j}k}{\Delta_y}\frac{z-1}{z+1}\right\}\Psi_m(z)=0. \qquad (84)$$

The solution to (84) can be in analogy to (37) and (38) written as

$$\Psi_{m+1}(z)=H(z)\Psi_m(z), \qquad (85)$$

where

$$H(z)=1+B(z)+\sqrt{2B(z)+B^2(z)} \qquad (86)$$

or in the impedance form

$$\Psi_m(z)=G(z)\left[\Psi_{m+1}(z)-\Psi_m(z)\right], \qquad (87)$$

where

$$G(z)=\left[B(z)+\sqrt{2B(z)+B^2(z)}\right]^{-1}. \qquad (88)$$

The term

$$B(z)=\frac{\Delta_x^2}{2}A(z), \qquad (89)$$

where $A(z)$ is given in (64), is identical with $B(p)$ in (39) with the relation (66) between p and z.

For the simple case of the homogeneous space, $k=\beta$, one obtains

$$B(z)=\frac{2\mathrm{j}k\Delta_x^2}{\Delta_y}\frac{z-1}{z+1}=2\Omega\frac{z-1}{z+1}, \qquad (90)$$

where $\Omega=\mathrm{j}k\Delta_x^2/\Delta_y$.

The inversion of (85) yields the convolution

$$\psi_{m+1}^N=\{h_n\}\otimes\left\{\psi_m^{N-n}\right\}=\sum_{n=0}^{N}h_n\psi_m^{N-n}, \qquad (91)$$

where $\{h_n\}_{n=0,1,2,..}$ is the inverse Z-transform sequence pertaining to the weighting function $H(z)$ in (86), i.e.

$$\sum_{n=0}^{\infty}h_n z^{-n}=1+B(z)+\sqrt{2B(z)+B^2(z)}. \qquad (92)$$

Similarly the inversion of (87) yields

$$\psi_m^N=\sum_{n=0}^{N}g_n\left(\psi_{m+1}^{N-n}-\psi_m^{N-n}\right), \qquad (93)$$

where

$$\sum_{n=0}^{\infty} g_n z^{-n} = \left[B(z) + \sqrt{2B(z) + B^2(z)} \right]^{-1} . \quad (94)$$

The analytical inversion of (92) has been obtained in [4] and is in a simplified form presented in Appendix 2. In [4] also a thorough analysis of various rather subtle mathematical aspects of the technique is presented. In a similar way the analytical inversion of (94) can be obtained too, and is also presented in Appendix 2.

In the spirit of the presented development the weighting function $G(z)$ in (87) can be recast similarly as in (48) into the form

$$G(z) = \frac{1}{\sqrt{2B(z)}} \left\{ \sqrt{1 + B(z)/2} - \sqrt{B(z)/2} \right\}, \quad (95)$$

and the similar development as in formulas (48)-(54) of Section 3 can be performed for the discrete convolution. For the intermediate result analogous to (53) of the first convolution pertaining to the weighting function $1/\sqrt{2B(z)}$ one obtains

$$\phi_m^N = \sqrt{\frac{\Delta_y}{4jk}} \sum_{n=0}^{N} a_n \frac{\psi_{m+1}^{N-n} - \psi_m^{N-n}}{\Delta_x}, \quad (96)$$

where $\{a_n\}_{n=0,1,2,..}$ is given in (70), i.e. (96) is the discrete pendant to (69).

The second discrete convolution analogous to (54) one obtains in the form

$$\psi_m^N = \sum_{n=0}^{N} d_n \phi_m^{N-n} \quad (97)$$

where

$$\sum_{n=0}^{\infty} d_n z^{-n} = \sqrt{1 + B(z)/2} - \sqrt{B(z)/2} . \quad (98)$$

Note that the sequence $\{d_n\}_{n=0,1,2,..}$ can be written as the subtraction of two sequences

$$\{d_n\}_{n=0,1,2,..} = \{s_n\}_{n=0,1,2,..} - \{r_n\}_{n=0,1,2,..} . \quad (99)$$

The sequence $\{s_n\}_{n=0,1,2,..}$

$$\sum_{n=0}^{\infty} s_n z^{-n} = \sqrt{1 + \Omega \frac{z-1}{z+1}} , \quad (100)$$

can be obtained numerically as outlined in Appendix 3 and its first few terms are

$$\{s_n\}\big|_{n=0,1,2,..} = \sqrt{1+\Omega} \Big\{ 1,\ -\gamma, \left[-\tfrac{1}{2}\gamma^2 + \gamma \right],$$

$$, \left[-\tfrac{1}{2}\gamma^3 + \gamma^2 - \gamma \right], \left[-\tfrac{5}{8}\gamma^4 + \tfrac{3}{2}\gamma^3 - \tfrac{3}{2}\gamma^2 + \gamma \right],$$

$$, \left[-\tfrac{7}{8}\gamma^5 + \tfrac{5}{2}\gamma^4 - 3\gamma^3 + 2\gamma^2 - \gamma \right],$$

$$, \left[-\tfrac{21}{16}\gamma^6 + \tfrac{35}{8}\gamma^5 - \tfrac{25}{4}\gamma^4 + 5\gamma^3 - \tfrac{5}{2}\gamma^2 + \gamma \right], \ldots \Big\}, \quad (101)$$

where $\gamma = \Omega/(1+\Omega)$. The second sequence $\{r_n\}_{n=0,1,2,..}$ can be with help of (70) written in the form

$$\{r_n\}_{n=0,1,2,..} = \sqrt{\Omega} \{b_n\}_{n=0,1,2,..} \quad (102)$$

where $\{b_n\}_{n=0,1,2,..}$ is again given by (70).

For the limiting case $\Omega \to 0$, i.e. for the transversal-discretisation-interval-length Δ_x converging to zero, $\Delta_x \to 0$, the sequence $\{d_n\}_{n=0,1,2,..}$ approaches the limit in the form of a delta-sequence (138)

$$\{d_n\}_{n=0,1,2,..} \approx \{1,0,0,0,0,..\}, \ \Delta_x \to 0 . \quad (103)$$

In this case , as it stems from (97), $\psi_m^N = \phi_m^N$ and ψ_m^N is equal to the discrete form (96) of the convolution formula (69) for the semi-discrete approach in the propagation direction.

On the other hand, for small steps in the propagation direction i.e $\Delta_y \ll k\Delta_x^2$, when Ω is large, $\Omega \gg 1$, the nominator in (95) can be approximated as

$$\sqrt{1 + B(z)/2} - \sqrt{B(z)/2} \approx \sqrt{1/2B(z)} , \quad (104)$$

Then the sequence $\{d_n\}_{n=0,1,2,..}$ in (97) is asymptotically identical with $\sqrt{\Delta_y / jk\Delta_x^2}\, \{a_n\}_{n=0,1,2,..}$

This asymptotics can be obtained directly from the asymptotic behaviour of $G(z)$ for $\Delta_y \ll k\Delta_x^2$

$$G(z) \approx 1/2B(z) = \frac{\Delta_y}{2\,jk\Delta_x^2} \frac{z+1}{z-1}, \quad (105)$$

yielding thus, using (142), the asymptotic expression for $\{g_n\}_{n=0,1,2,..}$ in the form

$$\{g_n\}_{n=0,1,2,..} \approx \frac{\Delta_y}{2\,jk\Delta_x^2} \{1,2,2,2,2,....\} . \quad (106)$$

7. NUMERICAL IMPLEMENTATION OF TBC IN THE CRANK-NICOLSON METHOD

For numerical simulations solely the full Crank-Nicolson formula (83) is used. It can be written in the form (where A, B, C, D, E, F are appropiate constants)

$$D\psi_2^{n+1} - E\psi_1^{n+1} =$$

$$= A\psi_2^n - B\psi_1^n + C\psi_0^n - F\psi_0^{n+1}, \quad (107)$$

$$D\psi_{m+1}^{n+1} - E\psi_m^{n+1} + F\psi_{m-1}^{n+1} =$$

$$= A\psi_{m+1}^n - B\psi_m^n + C\psi_{m-1}^n, \ m = 2, 3, ..., M-2, \quad (108)$$

$$-E\psi_{M-1}^{n+1} + F\psi_{M-2}^{n+1} =$$

$$= A\psi_M^n - B\psi_{M-1}^n + C\psi_{M-2}^n - D\psi_M^{n+1}, \quad (109)$$

i.e. the unknowns ψ_i^{n+1}, $i = 1, 2, ..., M-1$ on the left sides of (107)-(109) are expressed by the known values in the previous layer ψ_i^n, $i = 0, 1, 2, ..., M$ and by the "must-be-known" boundary values ψ_0^{n+1}, ψ_M^{n+1}. This is an implicit type of discretisation scheme, i.e. it requires the solution of a tridiagonal system of equations for each step in the propagation direction z.

All convolution-type formulas (for the continuous formulation after the suitable interpolation of discrete data and subsequent integration as outlined in Section 5) can be easily embodied within the Crank-Nicholson scheme. The values of continuous x-derivatives in (30) and in (69) must be in boundary points first approximated by their discrete counterparts

$$\partial\psi(x, y_n)/\partial x\big|_{x=0} \approx (\psi_1^n - \psi_0^n)/\Delta_x, \quad (110)$$

$$\partial\psi(x, y_n)/\partial x\big|_{x=x_{\max}} \approx (\psi_M^n - \psi_{M-1}^n)/\Delta_x. \quad (111)$$

From (110) and e.g. (69) one obtains for the "left" boundary

$$(1 + a_0\xi)\psi_0^{n+1} =$$

$$= a_0\xi\psi_1^{n+1} + \xi\sum_{i=1}^{n+1} a_i\left(\psi_1^{n+1-i} - \psi_0^{n+1-i}\right), \quad (112)$$

where $\xi = \sqrt{\Delta_y/4\mathrm{j}k\Delta_x^2}$. After having substituted into (107) one obtains instead of (107) the equation

$$D\psi_2^{n+1} + \left\{\frac{Fa_0\xi}{(1 + a_0\xi)} - E\right\}\psi_1^{n+1} =$$

$$= A\psi_2^n - B\psi_1^n + C\psi_0^n -$$

$$-F\frac{\xi}{(1 + a_0\xi)}\sum_{i=1}^{n+1}\left(\psi_1^{n+1-i} - \psi_0^{n+1-i}\right)a_i, \quad (113)$$

with only the known values on its right-hand-side.

Similar holds for the "right" boundary too, i.e. from (111) and (69)

$$(1 - a_0\xi)\psi_M^{n+1} =$$

$$= -a_0\xi\psi_{M-1}^{n+1} + \xi\sum_{i=1}^{n+1}\left(\psi_M^{n+1-i} - \psi_{M-1}^{n+1-i}\right)a_i. \quad (114)$$

The substitution into (109) yields the equation

$$-\left\{\frac{Da_0\xi}{(1 - a_0\xi)} - E\right\}\psi_{M-1}^{n+1} + F\psi_{M-2}^{n+1} = A\psi_2^n - B\psi_1^n +$$

$$+C\psi_0^n - D\frac{\xi}{(1 - a_0\xi)}\sum_{i=1}^{n+1}\left(\psi_M^{n+1-i} - \psi_{M-1}^{n+1-i}\right)a_i. \quad (115)$$

In both equations, (113) and (115), one has to use the correct branch of the $\sqrt{\mathrm{j}}$ for the outgoing wave.

As already mentioned the main drawback of all four above formulations is the non-locality of the boundary conditions, i.e. for the successful application of the TBC one has to keep track of all previous values $\psi_1^n - \psi_0^n$, $\psi_M^n - \psi_{M-1}^n$, for $n = 0, 1, 2, ... N-1$ up to the actually calculated layer $n = N$.

8. POWER CONSERVATION AND THE NUMERICAL DISPERSION

Let us consider the obliquely propagating plane wave as in (12)

$$\psi(x, y) = \exp(-\mathrm{j}q_x x)\exp(-\mathrm{j}\kappa y), \quad (116)$$

and the "dispersion relation" (13)

$$\kappa = (\beta^2 - k^2 - q_x^2)/2k. \quad (117)$$

If one takes the so called "amplification factor" ξ in the form $\xi = \exp(-\mathrm{j}\kappa\Delta_y)$ then the discretised plane wave reads

$$\psi(x_m, y_n) = \xi^n\exp(-\mathrm{j}q_x m\Delta_x), \quad (118)$$

where in an ideal case $\xi = \exp(-\mathrm{j}\kappa\Delta_y)$, i.e. the wave-power density is conserved since magnitude of the propagating-wave envelope is unity, $|\xi| = 1$. The exact phase shift after one step in propagation direction is

$$\mathrm{phase}(\xi) = -\kappa\Delta_y = -\frac{\beta^2 - k^2 - q_x^2}{2k}\Delta_y. \quad (119)$$

However, after the substitution of (118) into the Crank-Nicolson implementation of the discrete parabolic wave equation (83) one obtains

$$\xi = \frac{1 - \mathrm{j}\Theta}{1 + \mathrm{j}\Theta}, \quad (120)$$

where

$$\Theta = \frac{\Delta_y}{2k}\left\{\frac{\beta^2 - k^2}{2} - \frac{2\sin^2(q_x\Delta_x/2)}{\Delta_x^2}\right\}. \quad (121)$$

It is easily seen that $|\xi| = 1$ holds further, i.e. the wave power remains conserved, but the phase shift in one longitudinal step is given by

$$\text{phase}(\xi) =$$

$$= 2\arctan\left[\frac{\Delta_y}{2k}\left\{\frac{\beta^2 - k^2}{2} - \frac{2\sin^2(q_x\Delta_x/2)}{\Delta_x^2}\right\}\right] \quad (122)$$

and differs from the "should be" exact value (119). This different dependence of the phase of ξ on the spatial frequency q_x is generally termed "numerical dispersion". Generally the difference between "physical" dispersion relation (119) and "numerical" dispersion relation (122) leads to deterioration of the shape of the wave-amplitude envelope and thus it is a highly unwanted effect.

Only if $q_x\Delta_x \ll 1$ holds, the term $\sin^2(q_x\Delta_x/2)$ can be approximated as $\sin^2(q_x\Delta_x/2) \approx q_x^2\Delta_x^2/4$ yielding for (122)

$$\text{phase}(\xi) \approx -2\arctan\frac{\beta^2 - k^2 - q_x^2}{4k}\Delta_y \quad (123)$$

Moreover, if the argument of arctan function is small then its value approximately equals to its argument and (123) converges to (119). If $k \approx \beta$ then it turns out that the condition $q_x^2\Delta_y \ll k$ must be fulfilled

In accordance with the sampling theorem the maximum value $\sin(q_x\Delta_x/2) = 1$ is reached for $q_x|_{\max} = \pi/\Delta_x$, where $q_x|_{\max}$ denotes the maximum spatial frequency in the transversal direction of the wave profile $\psi(x,y)$ that can be represented by its sampled values with sampling interval Δ_x. This frequency component is always present due to e.g. noise of the rounding errors of digital computations. However, in order to achieve small numerical dispersion one has to take care that the significant spatial-frequency components of the transversal profile of the wave-amplitude-envelope fulfil the condition $q_x\Delta_x \ll 1$. The second condition $q_x^2\Delta_y \ll k$ can be rewritten in the form

$$\Delta_y \ll k\Delta_x^2. \quad (124)$$

Both these conditions together guarantee small numerical dispersion.

9. CONCLUSIONS

Let us summarize the results. The continuous TBC is formulated as the convolution

$$\psi(x,y) = \int_0^y \frac{\partial\psi(x,\zeta)}{\partial x} f(y-\zeta)d\zeta \quad (125)$$

where

$$f(y) = \frac{1}{\sqrt{2\mathrm{j}k\pi y}} \quad (126)$$

The TBC discretised in transversal direction x is formulated as the double convolution

$$\phi_m(y) = \int_0^y \frac{\psi_{m+1}(\zeta) - \psi_m(\zeta)}{\Delta_x} f(y-\zeta)d\zeta \quad (127)$$

$$\psi_m(y) = \int_0^y \phi_m(\zeta)d(y-\zeta)d\zeta \quad (128)$$

where.

$$d(y) = \Delta_x\sqrt{\mathrm{j}k}\,\frac{1-\exp\left(-2y/\mathrm{j}k\Delta_x^2\right)}{2y\sqrt{2\pi y}} \quad (129)$$

The TBC discretised in longitudinal direction y is formulated in terms of the discrete convolution

$$\psi_N(x) = \sqrt{\frac{\Delta_y}{4\mathrm{j}k}}\sum_{n=0}^{N} a_n \frac{\partial\psi_{N-n}(x)}{\partial x}, \quad (130)$$

where

$$\{a_n\} =$$

$$= \left\{1, 1, \frac{1}{2}, \frac{1}{2}, \frac{1\cdot 3}{2\cdot 4}, \frac{1\cdot 3}{2\cdot 4}, \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}, \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}, ..\right\} \quad (131)$$

The TBC discretised in both transversal and longitudinal direction is given by

$$\phi_m^N = \sqrt{\frac{\Delta_y}{4\mathrm{j}k}}\sum_{n=0}^{N} a_n \frac{\psi_{m+1}^{N-n} - \psi_m^{N-n}}{\Delta_x}, \quad (132)$$

$$\psi_m^N = \sum_{n=0}^{N} d_n \phi_m^{N-n} \quad (133)$$

with $\{d_n\}$ given by (99) - (102).

As it has been shown, the limiting case $\Delta_x \to 0$ for transversally discretised formulation in (127) and (128) leads to $d(y)$ in (129) converging to δ-function. Thus one arrives to asymptotically the same result as for the continuous TBC, cf. (125).

Similarly it has been shown that the semi-discrete formulation (130) discretised in longitudinal direction leads in the limiting case $\Delta_y \to 0$ to continuous formulation of the TBC (125), (126) too. Thus all three formulations are asymptotically identical.

Any numerical simulations can be realised only in the fully discretised form accordingly (83). The formulation of the TBC discretised in both, the transversal as well in the longitudinal direction (132) and (133), is in the limit $\Delta_x \to 0$ identical with the semi-discrete formulation (130) too, since the sequence $\{d_n\}_{n=0,1,2,..}$ in (133) converges in such a case to the δ-sequence. However, for the finite values Δ_x the behaviour of the TBC depends on the ratio $\Delta_y / k\Delta_x^2$.

As discussed in Section 8 to reach small numerical dispersion the condition (124) has to be met. It has been shown that in such a case the second convolution (97) cannot be neglected and fulfilling (124) means that in fact the sequence $\{g_n\}_{n=0,1,2,..}$ cannot be simply taken as dicretised formula (69) but the full formula

$$\psi_m^N = \sum_{n=0}^{N} g_n \left(\psi_{m+1}^{N-n} - \psi_m^{N-n}\right) \qquad (134)$$

must be used, where

$$g_n = \sqrt{\frac{\Delta_y}{4\,\mathrm{j}k\Delta_x^2}} \sum_{k=0}^{n} a_k d_{n-k}\,. \qquad (135)$$

As pointed out, the convolution (135) asymptotically leads to the sequence (106)

$$\{g_n\}_{n=0,1,2,..} \approx \frac{\Delta_y}{2\,\mathrm{j}k\Delta_x^2}\{1,2,2,2,2,....\}\,. \quad (136)$$

The use of any other formula, following from the continuous or semi-discrete formulation, not pertaining to the relation (124), is not consistent with the small numerical dispersion requirement. This represents the main new result of the theoretical analysis performed.

In the follow-up paper the results of comprehensive numerical simulations will be presented.

APPENDIX 1: SOME RULES AND PROPERTIES OF THE *Z*-TRANSFORM.

The *Z*-transform of the sequence $\{f_n\}_{n=0,1,2,..}$ is defined as

$$F(z) = \sum_{n=0}^{\infty} f_n z^{-n} \qquad (137)$$

Note that the values f_n in the *Z*-transform (137) are in fact the coefficients of the Taylor series expansion of the function $F(z)$ in the variable $1/z$.

Using some simple Taylor series expansions and power series sums It is easy to show validity of the following transform pairs

$$\{\delta_0\}_{n=0,1,2,..} = \{1,0,0,0,0,..\} \Leftrightarrow 1\,, \qquad (138)$$

$$\{\delta_1\}_{n=0,1,2,..} = \{0,1,0,0,0,..\} \Leftrightarrow \frac{1}{z}\,, \qquad (139)$$

$$\{1\}_{n=0,1,2,..} = \{1,1,1,1,1,..\} \Leftrightarrow \frac{z}{z-1}\,, \qquad (140)$$

where $\{\delta_0\}_{n=0,1,2,..}$ is the delta sequence $\{\delta_1\}_{n=0,1,2,..}$ the shifted delta sequence and $\{1\}_{n=0,1,2,..}$ is the unit-step sequence. Further

$$\{a^n\}_{n=0,1,2,..} \Leftrightarrow \frac{z}{z-a}\,, \qquad (141)$$

$$\{1,2,2,2,2,..\} \Leftrightarrow \frac{2z}{z-1} - 1 = \frac{z+1}{z-1} \qquad (142)$$

$$\{1,-2,2,-2,2,..\} \Leftrightarrow \frac{2z}{z+1} - 1 = \frac{z-1}{z+1} \qquad (143)$$

$$\left\{1, \pm 1, \frac{1}{2}, \pm\frac{1}{2}, \frac{1\cdot 3}{2\cdot 4}, \pm\frac{1\cdot 3}{2\cdot 4}, \frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}, \pm\frac{1\cdot 3\cdot 5}{2\cdot 4\cdot 6}, ..\right\} \Leftrightarrow$$

$$\Leftrightarrow \sqrt{\frac{z\pm 1}{z\mp 1}}\,. \qquad (144)$$

To the product

$$G(z) = F(z)H(z) \qquad (145)$$

in the Z-domain corresponds the discrete convolution of original sequences, i.e.

$$\{g_n\}_{n=0,1,2,..} = \{f_n\}_{n=0,1,2,..} \otimes \{h_n\}_{n=0,1,2,..}\,, \qquad (146)$$

expressed explicitly as

$$g_n = \sum_{k=0}^{n} f_{n-k} h_k = \sum_{k=0}^{n} f_k h_{n-k}\,. \quad (147)$$

If for the sequences $\{f_n\}_{n=0,1,2,..}$ and $\{g_n\}_{n=0,1,2,..}$

$$f_n = g_{n+1}\,,\; n = 0,1,2,... \qquad (148)$$

holds, then it is easy to show that for their *Z*-transforms the so called “shift theorem”

$$F(z) = zG(z)\,. \qquad (149)$$

holds.

APPENDIX 2: INVERSE TRANSFORM OF THE FORMULAE (86) AND (88).

The function $H(z)$ in (86) can be in case (90) expressed as

$$H(z)=1+\lambda\frac{z-1}{z+1}\pm\sqrt{\lambda\frac{z-1}{z+1}\left[\lambda\frac{z-1}{z+1}+2\right]},\quad(150)$$

where $\lambda=2\Omega=2\mathrm{j}k\Delta_x^2/\Delta_y$. This can easily be put in the form

$$H(z)=1+\lambda\left[\frac{2z}{z+1}-1\right]\pm$$

$$\pm\frac{\sqrt{\lambda}}{z+1}\sqrt{(\lambda+2)z^2-2\lambda z+\lambda-2}\,.\quad(151)$$

Further

$$\sqrt{(\lambda+2)z^2-2\lambda z+\lambda-2}=$$

$$=\frac{(\lambda+2)z^2-2\lambda z+\lambda-2}{z\sqrt{\lambda+2}}\frac{\mu z}{\sqrt{(\mu z)^2-2a\mu z+1}},\quad(152)$$

where $\mu=\sqrt{(\lambda+2)/(\lambda-2)}$ and $a=\sqrt{2\lambda/(\lambda^2-4)}$. Finally one obtains the formula

$$H(z)=(1-\lambda)+\lambda\frac{2z}{z+1}\pm$$

$$\pm\sqrt{\lambda-2}\left[\mu+\frac{1}{\mu z}+\frac{4a}{z+1}\right]\frac{\mu z}{\sqrt{(\mu z)^2-2a\mu z+1}},\quad(153)$$

Using the Z-transform pair

$$\{P_n(a)\}_{n=0,1,2,..}\Leftrightarrow\frac{z}{\sqrt{z^2-2az+1}},\quad(154)$$

where $P_n(a)$ are Legendre polynomials and results in Appendix 1, (153) can be back-transformed in the convolution form

$$\{h_n\}=(1-\lambda)\{\delta_0\}+2\lambda\left\{(-1)^n\right\}\pm$$

$$\pm\sqrt{\lambda-2}\left[\mu\{\delta_0\}+\frac{1}{\mu}\{\delta_1\}+4a\left(\left\{(-1)^n\right\}-\{\delta_0\}\right)\right]\otimes$$

$$\otimes\left\{\mu^{-n}P_n(a)\right\}.\quad(155)$$

Similarly $G(z)$ in (88) can be written as

$$G(z)=\frac{1}{2\lambda}\frac{z+1}{z-1}\sqrt{\lambda\frac{z-1}{z+1}\left[\lambda\frac{z-1}{z+1}+2\right]}-\frac{1}{2}\quad(156)$$

and recast into the form

$$G(z)=$$

$$=\left[K_1-\frac{K_2}{z-1}+\frac{K_3}{z}\right]\frac{\mu z}{\sqrt{(\mu z)^2-2a\mu z+1}}-\frac{1}{2},\quad(157)$$

where

$$K_1=\sqrt{\frac{\lambda+2}{4\lambda}},K_2=\sqrt{\frac{\lambda}{4\lambda+8}},K_3=\sqrt{\frac{1}{\lambda^2+2\lambda}}.\quad(158)$$

The sequence $\{g_n\}$ can be then easily obtained in an analogous way as the sequence $\{h_n\}$ in (155).

APPENDIX 3. INVERSE TRANSFORM OF THE FORMULA (100).

The sequence $\{s_n\}_{n=0,1,2,..}$ defined in (100) as

$$\sum_{n=0}^{\infty}s_nz^{-n}=\sqrt{1+\Omega\frac{z-1}{z+1}},\quad(159)$$

that represents the inverse Z-transform of $\sqrt{1+\Omega(z-1)/(z+1)}$, can be obtained as

$$s_n=\sqrt{\Omega}\frac{1}{n!}\frac{d^nf(\eta)}{d\eta^n}\bigg|_{\eta=0},\quad(160)$$

where $f(\eta)=\alpha^{1/2}$, $\alpha=\Omega^{-1}-1+2/\beta$, $\beta=1+\eta$.

The first and the second derivative of $f(\eta)$ are

$$f'(\eta)=D_{11}\alpha^{-1/2}\beta^{-2},\quad(161)$$

$$f''(\eta)=D_{21}\alpha^{-3/2}\beta^{-4}+D_{22}\alpha^{-1/2}\beta^{-3}\quad(162)$$

where

$$\begin{aligned}D_{11}&=-1\\D_{21}&=D_{11}=-1\\D_{22}&=-2D_{11}=2\end{aligned}\quad.\quad(163)$$

Further

$$f'''(\eta)=$$

$$=D_{31}\alpha^{-5/2}\beta^{-6}+D_{32}\alpha^{-3/2}\beta^{-5}+D_{33}\alpha^{-1/2}\beta^{-4}\quad(164)$$

where

$$\begin{aligned}D_{31}&=3D_{21}=-3\\D_{32}&=-4D_{21}+D_{22}=6\\D_{33}&=-3D_{22}=-6\end{aligned}\quad(165)$$

From the above one can infer the general recursive algorithm. If

$$f^{(n-1)}(\eta)=\sum_{k=1}^{n}D_{n-1,k}\alpha^{-(2n-2k-1)/2}\beta^{-(2n-k)}\quad(166)$$

then

$$f^{(n)}(\eta)=\sum_{k=1}^{n} D_{n,k}\alpha^{-(2n-2k+1)/2}\beta^{-(2n-k+1)} \quad (167)$$

where

$$\begin{aligned} &D_{n,1}=(2n-3)D_{n-1,1} \\ &D_{n,k}=(2n-2k-1)D_{n-1,k}- \\ &\qquad -(2n-k)D_{n-1,k-1},\ k=2,3,..,n-1 \\ &D_{n,n}=-nD_{n-1,n-1} \end{aligned} \quad (168)$$

The first few coefficients $D_{n,k}$ are summarized in Table 3.

Table 3. Values of $D_{n,k}$

n\k	1	2	3	4	5	6
1	-1					
2	-1	2				
3	-3	6	-6			
4	-15	36	-36	24		
5	-105	300	-360	240	-120	
6	-945	3150	-4500	3600	-1800	720

Substituting $\eta=0$ into respective derivatives $f^{(n)}(\eta)$, $n=1,2,3,..$ one obtains from (160) the sequence (101).

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