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РОССИЙСКАЯ АКАДЕМИЯ НАУК
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TRANSPARENT BOUNDARY CONDITIONS FOR 2D
MAXWELL EQUATIONS IN LORENTZ MEDIA

Москва, 2010

N.A. Zaitsev, I.L. Sofronov. *Transparent boundary conditions for 2D Maxwell equations in Lorentz media.*

Abstract. Transparent Boundary Conditions (TBCs) for 2D TE_y mode of Maxwell's equations in dispersive media described by Lorentz theory are proposed. Analytical formulas of TBCs contain a non-local term with convolutions with respect to time. In order to discretize TBCs for the alternate direction implicit time-stepping algorithm (ADI) derived in [1] for extended system we reformulate convolutions using auxiliary variables.

Н.А. Зайцев, И.Л. Софронов. *Прозрачные граничные условия для двумерных уравнений Максвелла в Лоренцевых средах.*

Аннотация. Рассмотрен случай TE_y моды двумерных уравнений Максвелла в средах с дисперсией, описываемой теорией Лоренца. Для плоской открытой границы выведены прозрачные граничные условия (ПГУ). Ядро свертки по времени, входящей в нелокальную часть оператора ПГУ, состоит из двух сумм экспонент: основной, определяемой волновым оператором и добавочной, определяемой сверточным оператором магнитной восприимчивости. Предложена дискретизация полученного оператора ПГУ в рамках схемы переменных направлений, применяемой для решения уравнений Максвелла внутри расчетной области.

Introduction

We propose transparent boundary conditions (TBCs) for 2D TE_y mode of Maxwell's equations in dispersive media described by Lorentz theory. Analytical formulas of TBCs contain a non-local term with convolutions with respect to time. In order to discretize TBCs for the alternate direction implicit time-stepping algorithm (ADI) derived in [1] for extended system we reformulate convolutions using auxiliary variables.

§1. TBC for the governing equations with convolution

Let us consider the TE_y mode of 2D Maxwell's equations for Lorentz media:

$$\begin{aligned} \frac{\partial D^x}{\partial t} &= -\frac{\partial H^y}{\partial z}, \\ \frac{\partial D^z}{\partial t} &= \frac{\partial H^y}{\partial x}, \\ \frac{\partial H^y}{\partial t} &= \frac{1}{\mu} \left(\frac{\partial E^z}{\partial x} - \frac{\partial E^x}{\partial z} \right), \\ \vec{D} &= \varepsilon_0 \varepsilon_\infty \vec{E} + \int_0^t \chi(\tau) \vec{E}(t-\tau) d\tau, \\ \chi(t) &= \text{Re} \left(\sum_{p=1}^P a_p e^{b_p t} \right). \end{aligned} \quad (1.1)$$

where \vec{E} is the electric field, \vec{H} is the magnetic field, \vec{D} is the electric flux density, $\varepsilon = \varepsilon_0 \varepsilon_\infty$ is the electrical permittivity, ε_0 is the free-space permittivity, ε_∞ is the relative permittivity at infinite frequency, $\mu = \mu_0 \mu_\infty$ is the magnetic permeability, χ is the real-valued susceptibility function approximated by a sum of exponentials (according to the Lorentz media).

Let the problem be L -periodic with respect to x , i.e.

$$u(x+L) = u(x)$$

for all functions u at any time. Denote by F_x the Fourier transform operator wrt x axis:

$$\hat{u}_\xi = F_x[u(x)] \quad (1.2)$$

Then (1.1) gives

$$\begin{aligned}
 \frac{\partial \hat{D}_\xi^x}{\partial t} &= -\frac{\partial \hat{H}_\xi^y}{\partial z}, \\
 \frac{\partial \hat{D}_\xi^z}{\partial t} &= i\xi \hat{H}_\xi^y, \\
 \frac{\partial \hat{H}_\xi^y}{\partial t} &= \frac{1}{\mu} \left(i\xi \hat{E}_\xi^z - \frac{\partial \hat{E}_\xi^x}{\partial z} \right), \\
 \vec{\hat{D}}_\xi &= \varepsilon_0 \varepsilon_\infty \vec{\hat{E}}_\xi + \varepsilon_0 \int_0^t \chi(\tau) \vec{\hat{E}}_\xi(t-\tau) d\tau, \\
 \chi(t) &= \operatorname{Re} \left(\sum_{p=1}^P a_p e^{b_p t} \right).
 \end{aligned} \tag{1.3}$$

Here μ is constant.

Laplace transformation of (1.3) reads

$$\begin{aligned}
 s \breve{D}_\xi^x &= -\frac{\partial \breve{H}_\xi^y}{\partial z}, \\
 s \breve{D}_\xi^z &= i\xi \breve{H}_\xi^y, \\
 s \breve{H}_\xi^y &= \frac{1}{\mu} \left(i\xi \breve{E}_\xi^z - \frac{\partial \breve{E}_\xi^x}{\partial z} \right), \\
 \vec{\breve{D}}_\xi &= \varepsilon_0 \varepsilon_\infty \vec{\breve{E}}_\xi + \varepsilon_0 \breve{\chi}(s) \vec{\breve{E}}_\xi(s), \\
 \breve{\chi}(s) &= \sum_{p=1}^P \frac{a_{r,p} (s - b_{r,p}) - a_{i,p} b_{i,p}}{(s - b_{r,p})^2 + b_{i,p}^2}
 \end{aligned} \tag{1.4}$$

where $a_p = a_{r,p} + ia_{i,p}$, $b_p = b_{r,p} + ib_{i,p}$, $a_{r,p}, a_{i,p}, b_{r,p}, b_{i,p} \in \mathbb{C}$. Here ε_0 and ε_∞ are constants. Let us eliminate $\vec{\breve{D}}_\xi$:

$$\begin{aligned}
s(\varepsilon_0 \varepsilon_\infty + \varepsilon_0 \check{\chi}(s)) \check{E}_\xi^x &= -\frac{\partial \check{H}_\xi^y}{\partial z}, \\
s(\varepsilon_0 \varepsilon_\infty + \varepsilon_0 \check{\chi}(s)) \check{E}_\xi^z &= i\xi \check{H}_\xi^y, \\
s \check{H}_\xi^y &= \frac{1}{\mu} \left(i\xi \check{E}_\xi^z - \frac{\partial \check{E}_\xi^x}{\partial z} \right).
\end{aligned} \tag{1.5}$$

After eliminating \check{E}_ξ^x and \check{E}_ξ^z we obtain

$$s^2 (\mu \varepsilon_0 \varepsilon_\infty + \mu \varepsilon_0 \check{\chi}(s)) \check{H}_\xi^y = \frac{\partial^2 \check{H}_\xi^y}{\partial z^2} - \xi^2 \check{H}_\xi^y. \tag{1.6}$$

Equation (1.6) is an equation of the form

$$u'' = au \tag{1.7}$$

where

$$a = s^2 (\mu \varepsilon_0 \varepsilon_\infty + \mu \varepsilon_0 \check{\chi}(s)) + \xi^2.$$

The generic solution of (1.7) is

$$u(z) = c_1 e^{\sqrt{a}z} + c_2 e^{-\sqrt{a}z}. \tag{1.8}$$

Decaying generic solutions are

$$u(z) = c e^{-\sqrt{a}z} \tag{1.9}$$

while $z \rightarrow +\infty$, and

$$u(z) = c e^{\sqrt{a}z} \tag{1.10}$$

while $z \rightarrow -\infty$. Hence for every solution decaying while $z \rightarrow +\infty$ the following relation holds:

$$u' = -\sqrt{a} u. \tag{1.11}$$

Similarly, for every solution decaying while $z \rightarrow -\infty$ the following relation holds:

$$u' = \sqrt{a} u. \tag{1.12}$$

Relations (1.11) and (1.12) give the TBCs we need in Fourier-Laplace space:

$$\frac{\partial \check{H}_\xi^y}{\partial z} + \sqrt{s^2 (\mu \varepsilon_0 \varepsilon_\infty + \mu \varepsilon_0 \check{\chi}(s)) + \xi^2} \check{H}_\xi^y = 0 \tag{1.13}$$

at the upper boundary, and

$$\frac{\partial \check{H}_\xi^y}{\partial z} - \sqrt{s^2 (\mu \varepsilon_0 \varepsilon_\infty + \mu \varepsilon_0 \check{\chi}(s)) + \xi^2} \check{H}_\xi^y = 0 \quad (1.14)$$

at the lower boundary.

Let ν be the outer normal to the top and the bottom boundaries. Then we write both equations (1.13) and (1.14) in a single form:

$$\frac{\partial \check{H}_\xi^y}{\partial \nu} + \sqrt{s^2 (\mu \varepsilon_0 \varepsilon_\infty + \mu \varepsilon_0 \check{\chi}(s)) + \xi^2} \check{H}_\xi^y = 0 \quad (1.15)$$

Subtracting the main term $s\sqrt{\mu \varepsilon_0 \varepsilon_\infty}$ from the root in (1.15) and making the inverse Laplace transform we get

$$\sqrt{\mu \varepsilon_0 \varepsilon_\infty} \frac{\partial \hat{H}_\xi^y}{\partial t} + \frac{\partial \hat{H}_\xi^y}{\partial \nu} + A(t, \xi) * \hat{H}_\xi^y = 0 \quad (1.16)$$

where

$$A(t, \xi) := L^{-1} \left[\sqrt{s^2 (\mu \varepsilon_0 \varepsilon_\infty + \mu \varepsilon_0 \check{\chi}(s)) + \xi^2} - s\sqrt{\mu \varepsilon_0 \varepsilon_\infty} \right] (t) \quad (1.17)$$

denotes the inverse Laplace transform of the kernel.

Recalling (1.2) we get the desired TBC for H^y :

$$\sqrt{\mu \varepsilon_0 \varepsilon_\infty} \frac{\partial H^y}{\partial t} + \frac{\partial H^y}{\partial \nu} + F_x^{-1} \{ A(t, \xi) * \} F_x H^y = 0. \quad (1.18)$$

§2. TBC for the governing equations in extended form

Instead of governing equations (1.1) we can start from equations (1.16)-(1.18) of [1] which for the TE_y mode read

$$\begin{aligned} \frac{\partial E^x}{\partial t} &= -\frac{1}{\varepsilon} \frac{\partial H^y}{\partial z} + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p P_p^x + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p Q_p^x - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p E^x, \\ \frac{\partial E^z}{\partial t} &= \frac{1}{\varepsilon} \frac{\partial H^y}{\partial x} + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p P_p^z + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p Q_p^z - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p E^z, \\ \frac{\partial H^y}{\partial t} &= \frac{1}{\mu} \left(\frac{\partial E^z}{\partial x} - \frac{\partial E^x}{\partial z} \right), \end{aligned}$$

$$\begin{aligned}
\frac{\partial P_p^x}{\partial t} &= -\alpha_p P_p^x - \beta_p Q_p^x + \delta_p E^x, \quad p = 1, \dots, P; \\
\frac{\partial P_p^z}{\partial t} &= -\alpha_p P_p^z - \beta_p Q_p^z + \delta_p E^z, \quad p = 1, \dots, P; \\
\frac{\partial Q_p^x}{\partial t} &= -\alpha_p Q_p^x + \beta_p P_p^x - \gamma_p E^x, \quad p = 1, \dots, P; \\
\frac{\partial Q_p^z}{\partial t} &= -\alpha_p Q_p^z + \beta_p P_p^z - \gamma_p E^z, \quad p = 1, \dots, P.
\end{aligned} \tag{2.1}$$

where

$$\begin{aligned}
a_p &= \delta_p - i\gamma_p, \\
b_p &= -\alpha_p + i\beta_p.
\end{aligned}$$

$\vec{P} = \sum_{p=1}^P \bar{P}_p$ is the electric polarization in the equation $\vec{D} = \epsilon_0 \epsilon_\infty \vec{E} + \vec{P}$; its components are represented in form $\tilde{P}_p = \vec{P}_p + i\vec{Q}_p$ after introducing auxiliary vectors $\vec{P}_p = \text{Re}(\tilde{P}_p)$ and $\vec{Q}_p = \text{Im}(\tilde{P}_p)$.

Fourier transform (1.2) gives:

$$\begin{aligned}
\frac{\partial \hat{E}_\xi^x}{\partial t} &= -\frac{1}{\epsilon} \frac{\partial \hat{H}_\xi^y}{\partial z} + \frac{1}{\epsilon_\infty} \sum_{p=1}^P \alpha_p \hat{P}_{p,\xi}^x + \frac{1}{\epsilon_\infty} \sum_{p=1}^P \beta_p \hat{Q}_{p,\xi}^x - \frac{1}{\epsilon_\infty} \sum_{p=1}^P \delta_p \hat{E}_\xi^x, \\
\frac{\partial \hat{E}_\xi^z}{\partial t} &= i\xi \frac{1}{\epsilon} \hat{H}_\xi^y + \frac{1}{\epsilon_\infty} \sum_{p=1}^P \alpha_p \hat{P}_{p,\xi}^z + \frac{1}{\epsilon_\infty} \sum_{p=1}^P \beta_p \hat{Q}_{p,\xi}^z - \frac{1}{\epsilon_\infty} \sum_{p=1}^P \delta_p \hat{E}_\xi^z, \\
\frac{\partial \hat{H}_\xi^y}{\partial t} &= \frac{1}{\mu} \left(i\xi \hat{E}_\xi^z - \frac{\partial \hat{E}_\xi^x}{\partial z} \right), \\
\frac{\partial \hat{P}_{p,\xi}^x}{\partial t} &= -\alpha_p \hat{P}_{p,\xi}^x - \beta_p \hat{Q}_{p,\xi}^x + \delta_p \hat{E}_\xi^x, \quad p = 1, \dots, P; \\
\frac{\partial \hat{P}_{p,\xi}^z}{\partial t} &= -\alpha_p \hat{P}_{p,\xi}^z - \beta_p \hat{Q}_{p,\xi}^z + \delta_p \hat{E}_\xi^z, \quad p = 1, \dots, P;
\end{aligned} \tag{2.2}$$

$$\frac{\partial \hat{Q}_{p,\xi}^x}{\partial t} = -\alpha_p \hat{Q}_{p,\xi}^x + \beta_p \hat{P}_{p,\xi}^x - \gamma_p \hat{E}_\xi^x, \quad p=1,...,P;$$

$$\frac{\partial \hat{Q}_{p,\xi}^z}{\partial t} = -\alpha_p \hat{Q}_{p,\xi}^z + \beta_p \hat{P}_{p,\xi}^z - \gamma_p \hat{E}_\xi^z, \quad p=1,...,P.$$

The Laplace transform gives:

$$\begin{aligned}
s\check{E}_\xi^x &= -\frac{1}{\varepsilon} \frac{\partial \check{H}_\xi^y}{\partial z} + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p \check{P}_{p,\xi}^x + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p \check{Q}_{p,\xi}^x - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p \check{E}_\xi^x, \\
s\check{E}_\xi^z &= \frac{i\xi}{\varepsilon} \check{H}_\xi^y + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p \check{P}_{p,\xi}^z + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p \check{Q}_{p,\xi}^z - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p \check{E}_\xi^z, \\
s\check{H}_\xi^y &= \frac{1}{\mu} \left(i\xi \check{E}_\xi^z - \frac{\partial \check{E}_\xi^x}{\partial z} \right), \\
s\check{P}_{p,\xi}^x &= -\alpha_p \check{P}_{p,\xi}^x - \beta_p \check{Q}_{p,\xi}^x + \delta_p \check{E}_\xi^x, \quad p=1,...,P; \tag{2.3} \\
s\check{P}_{p,\xi}^z &= -\alpha_p \check{P}_{p,\xi}^z - \beta_p \check{Q}_{p,\xi}^z + \delta_p \check{E}_\xi^z, \quad p=1,...,P; \\
s\check{Q}_{p,\xi}^x &= -\alpha_p \check{Q}_{p,\xi}^x + \beta_p \check{P}_{p,\xi}^x - \gamma_p \check{E}_\xi^x, \quad p=1,...,P; \\
s\check{Q}_{p,\xi}^z &= -\alpha_p \check{Q}_{p,\xi}^z + \beta_p \check{P}_{p,\xi}^z - \gamma_p \check{E}_\xi^z, \quad p=1,...,P.
\end{aligned}$$

For each p from (2.3) follows:

$$\begin{aligned}
\check{P}_{p,\xi}^x &= \frac{\delta_p (s + \alpha_p) + \gamma_p \beta_p}{(s + \alpha_p)^2 + \beta_p^2} \check{E}_\xi^x, \\
\check{P}_{p,\xi}^z &= \frac{\delta_p (s + \alpha_p) + \gamma_p \beta_p}{(s + \alpha_p)^2 + \beta_p^2} \check{E}_\xi^z, \tag{2.4} \\
\check{Q}_{p,\xi}^x &= \frac{\beta_p \delta_p - \gamma_p (s + \alpha_p)}{(s + \alpha_p)^2 + \beta_p^2} \check{E}_\xi^x, \\
\check{Q}_{p,\xi}^z &= \frac{\beta_p \delta_p - \gamma_p (s + \alpha_p)}{(s + \alpha_p)^2 + \beta_p^2} \check{E}_\xi^z.
\end{aligned}$$

Hence

$$s\breve{E}_\xi^x = -\frac{1}{\varepsilon} \frac{\partial \breve{H}_\xi^y}{\partial z} + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \left[\alpha_p \frac{\delta_p(s+\alpha_p) + \gamma_p \beta_p}{(s+\alpha_p)^2 + \beta_p^2} + \beta_p \frac{\beta_p \delta_p - \gamma_p(s+\alpha_p)}{(s+\alpha_p)^2 + \beta_p^2} - \delta_p \right] \breve{E}_\xi^x,$$

$$s\breve{E}_\xi^z = \frac{i\xi}{\varepsilon} \breve{H}_\xi^y + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \left[\alpha_p \frac{\delta_p(s+\alpha_p) + \gamma_p \beta_p}{(s+\alpha_p)^2 + \beta_p^2} + \beta_p \frac{\beta_p \delta_p - \gamma_p(s+\alpha_p)}{(s+\alpha_p)^2 + \beta_p^2} - \delta_p \right] \breve{E}_\xi^z,$$

$$s\breve{H}_\xi^y = \frac{1}{\mu} \left(i\xi \breve{E}_\xi^z - \frac{\partial \breve{E}_\xi^x}{\partial z} \right).$$

Let us eliminate \breve{E}_ξ^x and \breve{E}_ξ^z :

$$\begin{aligned} & \left\{ s - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \left[\alpha_p \frac{\delta_p(s+\alpha_p) + \gamma_p \beta_p}{(s+\alpha_p)^2 + \beta_p^2} + \beta_p \frac{\beta_p \delta_p - \gamma_p(s+\alpha_p)}{(s+\alpha_p)^2 + \beta_p^2} - \delta_p \right] \right\} \breve{E}_\xi^x = -\frac{1}{\varepsilon} \frac{\partial \breve{H}_\xi^y}{\partial z}, \\ & \left\{ s - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \left[\alpha_p \frac{\delta_p(s+\alpha_p) + \gamma_p \beta_p}{(s+\alpha_p)^2 + \beta_p^2} + \beta_p \frac{\beta_p \delta_p - \gamma_p(s+\alpha_p)}{(s+\alpha_p)^2 + \beta_p^2} - \delta_p \right] \right\} \breve{E}_\xi^z = \frac{i\xi}{\varepsilon} \breve{H}_\xi^y, \\ & s \left\{ s - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \left[\alpha_p \frac{\delta_p(s+\alpha_p) + \gamma_p \beta_p}{(s+\alpha_p)^2 + \beta_p^2} + \beta_p \frac{\beta_p \delta_p - \gamma_p(s+\alpha_p)}{(s+\alpha_p)^2 + \beta_p^2} - \delta_p \right] \right\} \breve{H}_\xi^y \\ & = \frac{1}{\mu} i\xi \left\{ s - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \left[\alpha_p \frac{\delta_p(s+\alpha_p) + \gamma_p \beta_p}{(s+\alpha_p)^2 + \beta_p^2} + \beta_p \frac{\beta_p \delta_p - \gamma_p(s+\alpha_p)}{(s+\alpha_p)^2 + \beta_p^2} - \delta_p \right] \right\} \breve{E}_\xi^z \\ & - \frac{1}{\mu} \left\{ s - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \left[\alpha_p \frac{\delta_p(s+\alpha_p) + \gamma_p \beta_p}{(s+\alpha_p)^2 + \beta_p^2} + \beta_p \frac{\beta_p \delta_p - \gamma_p(s+\alpha_p)}{(s+\alpha_p)^2 + \beta_p^2} - \delta_p \right] \right\} \frac{\partial \breve{E}_\xi^x}{\partial z}. \end{aligned}$$

Hence

$$\begin{aligned}
& s \left\{ s - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \left[\alpha_p \frac{\delta_p(s + \alpha_p) + \gamma_p \beta_p}{(s + \alpha_p)^2 + \beta_p^2} + \beta_p \frac{\beta_p \delta_p - \gamma_p(s + \alpha_p)}{(s + \alpha_p)^2 + \beta_p^2} - \delta_p \right] \right\} \bar{H}_\xi^y \\
& = -\frac{\xi^2}{\varepsilon \mu} \bar{H}_\xi^y + \frac{1}{\varepsilon \mu} \frac{\partial^2 \bar{H}_\xi^y}{\partial z^2}.
\end{aligned}$$

or

$$\begin{aligned}
& s \left\{ \mu \varepsilon_0 \varepsilon_\infty s - \mu \varepsilon_0 \sum_{p=1}^P \left[\alpha_p \frac{\delta_p(s + \alpha_p) + \gamma_p \beta_p}{(s + \alpha_p)^2 + \beta_p^2} + \beta_p \frac{\beta_p \delta_p - \gamma_p(s + \alpha_p)}{(s + \alpha_p)^2 + \beta_p^2} - \delta_p \right] \right\} \bar{H}_\xi^y \\
& = \frac{\partial^2 \bar{H}_\xi^y}{\partial z^2} - \xi^2 \bar{H}_\xi^y.
\end{aligned} \tag{2.5}$$

In more usual notation the equation (2.5) reads

$$\begin{aligned}
& \frac{\partial^2 \bar{H}_\xi^y}{\partial z^2} - \xi^2 \bar{H}_\xi^y = \mu \varepsilon_0 \varepsilon_\infty s^2 \bar{H}_\xi^y \\
& + \mu \varepsilon_0 s \sum_{p=1}^P \left[b_{r,p} \frac{a_{r,p}(s - b_{r,p}) - a_{i,p}b_{i,p}}{(s - b_{r,p})^2 + b_{i,p}^2} - b_{i,p} \frac{b_{i,p}a_{r,p} + a_{i,p}(s - b_{r,p})}{(s - b_{r,p})^2 + b_{i,p}^2} + a_{r,p} \right] \bar{H}_\xi^y
\end{aligned} \tag{2.6}$$

Evidently, equation (2.6) coincides with (1.6). Indeed,

$$\begin{aligned}
\bar{\chi}(s) &= \sum_{p=1}^P \frac{a_{r,p}(s - b_{r,p}) - a_{i,p}b_{i,p}}{(s - b_{r,p})^2 + b_{i,p}^2} \\
s \bar{\chi}(s) &= s \sum_{p=1}^P \frac{a_{r,p}(s - b_{r,p}) - a_{i,p}b_{i,p}}{(s - b_{r,p})^2 + b_{i,p}^2} = \sum_{p=1}^P \frac{s \left[a_{r,p}(s - b_{r,p}) - a_{i,p}b_{i,p} \right]}{(s - b_{r,p})^2 + b_{i,p}^2} \\
&= \sum_{p=1}^P \left\{ \frac{s \left[a_{r,p}(s - b_{r,p}) - a_{i,p}b_{i,p} \right] - a_{r,p} \left[(s - b_{r,p})^2 + b_{i,p}^2 \right]}{(s - b_{r,p})^2 + b_{i,p}^2} + a_{r,p} \right\} \\
&= \sum_{p=1}^P \left\{ \frac{(a_{r,p}b_{r,p} - a_{i,p}b_{i,p})(s - b_{r,p}) - (a_{r,p}b_{i,p} + a_{i,p}b_{r,p})b_{i,p}}{(s - b_{r,p})^2 + b_{i,p}^2} + a_{r,p} \right\}
\end{aligned}$$

Thus we have shown that TBCs for both “extended” and “with convolutions” Maxwell equations describing Lorentz media are derived from equivalent equations. This is a confirmation of TBCs formulas.

§3. Reformulation of the TBCs using extended system

In order to calculate the convolution in the TBCs

$$\sqrt{\mu\epsilon_0\epsilon_\infty} \frac{\partial \hat{H}_\xi^y}{\partial t} + \frac{\partial \hat{H}_\xi^y}{\partial \nu} + A(t, \xi) * \hat{H}_\xi^y = 0$$

efficiently we have to approximate kernel A by a sum of exponentials

$$A(t, \xi) \approx \sum_{l=1}^{L(\xi)} \operatorname{Re} \left(a_{l,\xi} e^{b_{l,\xi} t} \right). \quad (3.1)$$

Let us have such approximation. Then we can rewrite the boundary condition in the following form:

$$\sqrt{\mu\epsilon_0\epsilon_\infty} \frac{\partial H^y}{\partial t} + \frac{\partial H^y}{\partial \nu} + F_x^{-1} \left\{ \sum_{l=1}^{\max L(\xi)} \operatorname{Re} \left(a_{l,\xi} e^{b_{l,\xi} t} \right) * \right\} F_x H^y = 0 \quad (3.2)$$

where F_x denotes the Fourier transform. In order to eliminate the convolution we introduce auxiliary functions $P_l(t, x)$ such that TBC (3.2) is equivalent to the following equation:

$$\sqrt{\mu\epsilon_0\epsilon_\infty} \frac{\partial H^y}{\partial t} + \nu \frac{\partial H^y}{\partial z} + \sum_{l=1}^{\max L(\xi)} P_l = 0 \quad (3.3)$$

where $\nu = 1$ for the upper boundary, and $\nu = -1$ for the lower one. Let's derive equations for $P_l(t, x)$. The Fourier transform of (3.3) yields

$$\sqrt{\mu\epsilon_0\epsilon_\infty} \frac{\partial \hat{H}_\xi^y}{\partial t} + \nu \frac{\partial \hat{H}_\xi^y}{\partial z} + \sum_{l=1}^L \hat{P}_{l,\xi} = 0 \quad (3.4)$$

where L denotes $\max_\xi L(\xi)$ and $\hat{P}_{l,\xi}$ denotes the ξ th Fourier harmonic of the l th function:

$$\hat{P}_l = F_x P_l.$$

It follows from the comparison of equations (3.4) and (3.2) that

$$\hat{P}_{l,\xi} = \operatorname{Re}\left(a_{l,\xi} e^{b_{l,\xi} t}\right) * \hat{H}_{\xi}^y = \int_0^t \operatorname{Re}\left(a_{l,\xi} e^{b_{l,\xi} s}\right) \hat{H}_{\xi}^y(t-s) ds. \quad (3.5)$$

The upper limit is equal to t because all electro-magnetic functions are equal to zero for all $t < 0$. In addition we introduce functions

$$\tilde{P}_{l,\xi} = \left(a_{l,\xi} e^{b_{l,\xi} t}\right) * \hat{H}_{\xi}^y = \int_0^t a_{l,\xi} e^{b_{l,\xi} s} \hat{H}_{\xi}^y(t-s) ds = \int_0^t a_{l,\xi} e^{b_{l,\xi}(t-s)} \hat{H}_{\xi}^y(s) ds. \quad (3.6)$$

Evidently, $\tilde{P}_{l,\xi}$ satisfies the following equation:

$$\frac{\partial \tilde{P}_{l,\xi}}{\partial t} = a_{l,\xi} \hat{H}_{\xi}^y + b_{l,\xi} \tilde{P}_{l,\xi} \quad (3.7)$$

or for real functions

$$\begin{aligned} \frac{\partial \hat{P}_{l,\xi}}{\partial t} &= a_{l,\xi}^r \hat{H}_{\xi}^y + b_{l,\xi}^r \hat{P}_{l,\xi} - b_{l,\xi}^i \hat{Q}_{l,\xi}, \\ \frac{\partial \hat{Q}_{l,\xi}}{\partial t} &= a_{l,\xi}^i \hat{H}_{\xi}^y + b_{l,\xi}^i \hat{P}_{l,\xi} + b_{l,\xi}^r \hat{Q}_{l,\xi} \end{aligned} \quad (3.8)$$

where

$$\tilde{P}_{l,\xi} = \hat{P}_{l,\xi} + i \hat{Q}_{l,\xi}; \quad a_{l,\xi} = a_{l,\xi}^r + i a_{l,\xi}^i; \quad b_{l,\xi} = b_{l,\xi}^r + i b_{l,\xi}^i.$$

We can rewrite (3.8) thinking of $\hat{P}_l, \hat{Q}_l, \hat{E}$ as N_x -dimensional vectors:

$$\left. \begin{aligned} \frac{\partial \hat{P}_l}{\partial t} &= D_l^{a,r} \hat{H}^y + D_l^{b,r} \hat{P}_l - D_l^{b,i} \hat{Q}_l \\ \frac{\partial \hat{Q}_l}{\partial t} &= D_l^{a,i} \hat{H}_{\xi}^y + D_l^{b,i} \hat{P}_l + D_l^{b,r} \hat{Q}_l \end{aligned} \right\} \quad l = 1, \dots, L. \quad (3.9)$$

The diagonal matrices $D_l^{a,r}$, $D_l^{a,i}$, $D_l^{b,r}$ and $D_l^{b,i}$ are determined as follows:

$$\begin{aligned} \left(D_l^{a,r}\right)_{k,m} &= \delta_{k,m} a_{l,k}^r, & \left(D_l^{a,i}\right)_{k,m} &= \delta_{k,m} a_{l,k}^i, \\ \left(D_l^{b,r}\right)_{k,m} &= \delta_{k,m} b_{l,k}^r, & \left(D_l^{b,i}\right)_{k,m} &= \delta_{k,m} b_{l,k}^i. \end{aligned} \quad (3.10)$$

Here $\delta_{k,m}$ is the Kronecker symbol.

The inverse Fourier transform yields

$$\left. \begin{aligned} \frac{\partial P_l}{\partial t} &= F_x^{-1} D_l^{a,r} F_x H^y + F_x^{-1} D_l^{b,r} F_x P_l - F_x^{-1} D_l^{b,i} F_x Q_l \\ \frac{\partial Q_l}{\partial t} &= F_x^{-1} D_l^{a,i} F_x H^y + F_x^{-1} D_l^{b,i} F_x P_l + F_x^{-1} D_l^{b,r} F_x Q_l \end{aligned} \right\} \quad l = 1, \dots, L. \quad (3.11)$$

For the discrete Fourier transform with respect to x matrices F_x and F_x^{-1} read

$$\left(F_x\right)_{\xi j} = \frac{2\pi}{N_x} e^{-i\frac{2\pi}{N_x}\xi j}, \quad \left(F_x^{-1}\right)_{j\xi} = \frac{1}{2\pi} e^{i\frac{2\pi}{N_x}\xi j}. \quad (3.12)$$

After introducing matrices

$$\begin{aligned} A_l^{x,r} &= F_x^{-1} D_l^{a,r} F_x, & A_l^{x,i} &= F_x^{-1} D_l^{a,i} F_x, \\ B_l^{x,r} &= F_x^{-1} D_l^{b,r} F_x, & B_l^{x,i} &= F_x^{-1} D_l^{b,i} F_x, \end{aligned} \quad (3.13)$$

equation (3.11) reads

$$\left. \begin{aligned} \frac{\partial P_l}{\partial t} &= A_l^{x,r} H^y + B_l^{x,r} P_l - B_l^{x,i} Q_l \\ \frac{\partial Q_l}{\partial t} &= A_l^{x,i} H^y + B_l^{x,i} P_l + B_l^{x,r} Q_l \end{aligned} \right\} \quad l = 1, \dots, L. \quad (3.14)$$

These equations together with equation

$$\sqrt{\mu \epsilon_0 \epsilon_\infty} \frac{\partial H^y}{\partial t} + \nu \frac{\partial H^y}{\partial z} + \sum_{l=1}^L P_l = 0 \quad (3.15)$$

are equivalent to the TBC (3.2).

Remark 1. The TBC (3.2) (and hence (3.15), (3.14)) is not unique for Maxwell system. One can derive similar relations to other combinations of unknown functions.

Remark 2. The matrices (3.13) differ from the Fourier differentiation matrices only in diagonal factors: the last one has instead of $D_l^{a,r}$, for an example, the matrix

$$(D^x)_{k,m} = ik\delta_{k,m}.$$

§4. Implementation of TBCs for ADI

In order to incorporate TBCs into our hyperbolic problem we pass to the characteristic form of the equations and to replace characteristic relations along the incoming characteristic by appropriate formulas of (3.15), (3.14) for the same qualities (“invariants” that “propagate” along the characteristic) at the boundary. The characteristic form of system (2.1) with respect to z reads

$$\begin{aligned} \frac{\partial}{\partial t}(\sqrt{\varepsilon}E^x + \sqrt{\mu}H^y) + \frac{1}{\sqrt{\mu\varepsilon}}\frac{\partial}{\partial z}(\sqrt{\varepsilon}E^x + \sqrt{\mu}H^y) - \frac{1}{\sqrt{\mu}}\frac{\partial E^z}{\partial x} \\ = \frac{1}{\sqrt{\varepsilon}}\left(\frac{1}{\varepsilon_\infty}\sum_{p=1}^P \alpha_p P_p^x + \frac{1}{\varepsilon_\infty}\sum_{p=1}^P \beta_p Q_p^x - \frac{1}{\varepsilon_\infty}\sum_{p=1}^P \delta_p E^x\right), \end{aligned} \quad (4.1)$$

$$\begin{aligned} \frac{\partial}{\partial t}(\sqrt{\varepsilon}E^x - \sqrt{\mu}H^y) - \frac{1}{\sqrt{\mu\varepsilon}}\frac{\partial}{\partial z}(\sqrt{\varepsilon}E^x - \sqrt{\mu}H^y) + \frac{1}{\sqrt{\mu}}\frac{\partial E^z}{\partial x} \\ = \frac{1}{\sqrt{\varepsilon}}\left(\frac{1}{\varepsilon_\infty}\sum_{p=1}^P \alpha_p P_p^x + \frac{1}{\varepsilon_\infty}\sum_{p=1}^P \beta_p Q_p^x - \frac{1}{\varepsilon_\infty}\sum_{p=1}^P \delta_p E^x\right), \end{aligned} \quad (4.2)$$

$$\frac{\partial E^z}{\partial t} = \frac{1}{\varepsilon}\frac{\partial H^y}{\partial x} + \frac{1}{\varepsilon_\infty}\sum_{p=1}^P \alpha_p P_p^z + \frac{1}{\varepsilon_\infty}\sum_{p=1}^P \beta_p Q_p^z - \frac{1}{\varepsilon_\infty}\sum_{p=1}^P \delta_p E^z, \quad (4.3)$$

$$\begin{aligned} \frac{\partial P_p^x}{\partial t} &= -\alpha_p P_p^x - \beta_p Q_p^x + \delta_p E^x, \quad p = 1, \dots, P; \\ \frac{\partial P_p^z}{\partial t} &= -\alpha_p P_p^z - \beta_p Q_p^z + \delta_p E^z, \quad p = 1, \dots, P; \\ \frac{\partial Q_p^x}{\partial t} &= -\alpha_p Q_p^x + \beta_p P_p^x - \gamma_p E^x, \quad p = 1, \dots, P; \\ \frac{\partial Q_p^z}{\partial t} &= -\alpha_p Q_p^z + \beta_p P_p^z - \gamma_p E^z, \quad p = 1, \dots, P; \end{aligned} \quad (4.4)$$

where

$$\begin{aligned} a_p &= \delta_p - i\gamma_p, \\ b_p &= -\alpha_p + i\beta_p. \end{aligned}$$

Equation (4.1) corresponds to the eigenvalue $1/\sqrt{\mu\varepsilon}$, and equation (4.2) corresponds to the eigenvalue $-1/\sqrt{\mu\varepsilon}$. Hence at the upper boundary $z = z_{\max}$ one has to replace equation (4.2) by a boundary condition, and at the lower boundary $z = z_{\min}$ one has to replace equation (4.1) by another boundary condition. But usually such strict way is redundant. It seems more expedient to use the TBC (3.14) – (3.15) coupled with the following subsystem of (2.1) at z -boundaries:

$$\begin{aligned} \frac{\partial E^x}{\partial t} &= -\frac{1}{\varepsilon} \frac{\partial H^y}{\partial z} + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p P_p^x + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p Q_p^x - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p E^x, \\ \frac{\partial E^z}{\partial t} &= \frac{1}{\varepsilon} \frac{\partial H^y}{\partial x} + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p P_p^z + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p Q_p^z - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p E^z, \\ \frac{\partial P_p^x}{\partial t} &= -\alpha_p P_p^x - \beta_p Q_p^x + \delta_p E^x, \quad p = 1, \dots, P; \\ \frac{\partial P_p^z}{\partial t} &= -\alpha_p P_p^z - \beta_p Q_p^z + \delta_p E^z, \quad p = 1, \dots, P; \\ \frac{\partial Q_p^x}{\partial t} &= -\alpha_p Q_p^x + \beta_p P_p^x - \gamma_p E^x, \quad p = 1, \dots, P; \\ \frac{\partial Q_p^z}{\partial t} &= -\alpha_p Q_p^z + \beta_p P_p^z - \gamma_p E^z, \quad p = 1, \dots, P. \end{aligned} \tag{4.5}$$

We have to put $\nu = 1$ in (3.15) for the upper boundary, and $\nu = -1$ for the lower one.

In order to make use of the ADI for the system we rewrite it as follows:

$$\frac{\partial u}{\partial t} = Au + Bu \tag{4.6}$$

where $u = (E^x, H^y, E^z, P_p^x, Q_p^x, P_p^z, Q_p^z, P_l, Q_l)^T$. Functions $E^x, H^y, E^z, P_p^x, Q_p^x, P_p^z, Q_p^z$ are defined at all points, whereas functions P_l, Q_l are defined at the boundary points $z = z_{\min}$ and $z = z_{\max}$ only. At the inner points the system (4.6) coincides with the system (2.1) that reads

$$\frac{\partial E^x}{\partial t} = -\frac{1}{\varepsilon} \frac{\partial H^y}{\partial z} + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p P_p^x + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p Q_p^x - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p E^x, \tag{4.7}$$

$$\frac{\partial H^y}{\partial t} = \frac{1}{\mu} \frac{\partial E^z}{\partial x} - \frac{1}{\mu} \frac{\partial E^x}{\partial z}, \quad (4.8)$$

$$\frac{\partial E^z}{\partial t} = \frac{1}{\varepsilon} \frac{\partial H^y}{\partial x} + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p P_p^z + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p Q_p^z - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p E^z, \quad (4.9)$$

$$\begin{aligned} \frac{\partial P_p^x}{\partial t} &= -\alpha_p P_p^x - \beta_p Q_p^x + \delta_p E^x, \quad p = 1, \dots, P; \\ \frac{\partial Q_p^x}{\partial t} &= -\alpha_p Q_p^x + \beta_p P_p^x - \gamma_p E^x, \quad p = 1, \dots, P; \end{aligned} \quad (4.10)$$

$$\begin{aligned} \frac{\partial P_p^z}{\partial t} &= -\alpha_p P_p^z - \beta_p Q_p^z + \delta_p E^z, \quad p = 1, \dots, P; \\ \frac{\partial Q_p^z}{\partial t} &= -\alpha_p Q_p^z + \beta_p P_p^z - \gamma_p E^z, \quad p = 1, \dots, P. \end{aligned} \quad (4.11)$$

We assign to Au -part the following terms:

- in equation (4.7): $\frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p P_p^x + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p Q_p^x - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p E^x$
- in equation (4.8): $\frac{1}{\mu} \frac{\partial E^z}{\partial x}$
- in equation (4.9): $\frac{1}{\varepsilon} \frac{\partial H^y}{\partial x} + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p P_p^z + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p Q_p^z - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p E^z$
 $-\alpha_p P_p^x - \beta_p Q_p^x + \delta_p E^x, \quad p = 1, \dots, P;$
- in equation (4.10):
 $-\alpha_p Q_p^x + \beta_p P_p^x - \gamma_p E^x, \quad p = 1, \dots, P;$
 $-\alpha_p P_p^z - \beta_p Q_p^z + \delta_p E^z, \quad p = 1, \dots, P;$
- in equation (4.11):
 $-\alpha_p Q_p^z + \beta_p P_p^z - \gamma_p E^z, \quad p = 1, \dots, P.$

We assign to Bu -part the following terms:

- in equation (4.7): $-\frac{1}{\varepsilon} \frac{\partial H^y}{\partial z}$

- in equation (4.8): $-\frac{1}{\mu} \frac{\partial E^x}{\partial z}$
- in equation (4.9): nothing
- in equation (4.10): nothing
- in equation (4.11): nothing.

At the boundary points system (4.6) coincides with the system (4.7) – (4.11) with the only discrimination: equation (4.8) is replaced with equations (3.14) – (3.15). So it reads:

$$\frac{\partial E^x}{\partial t} = -\frac{1}{\varepsilon} \frac{\partial H^y}{\partial z} + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p P_p^x + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p Q_p^x - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p E^x, \quad (4.12)$$

$$\frac{\partial H^y}{\partial t} = \frac{-\nu}{\sqrt{\mu \varepsilon_0 \varepsilon_\infty}} \frac{\partial H^y}{\partial z} - \frac{1}{\sqrt{\mu \varepsilon_0 \varepsilon_\infty}} \sum_{l=1}^L P_l \quad (4.13)$$

$$\frac{\partial E^z}{\partial t} = \frac{1}{\varepsilon} \frac{\partial H^y}{\partial x} + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p P_p^z + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p Q_p^z - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p E^z, \quad (4.14)$$

$$\frac{\partial P_p^x}{\partial t} = -\alpha_p P_p^x - \beta_p Q_p^x + \delta_p E^x, \quad p = 1, \dots, P; \quad (4.15)$$

$$\frac{\partial Q_p^x}{\partial t} = -\alpha_p Q_p^x + \beta_p P_p^x - \gamma_p E^x, \quad p = 1, \dots, P;$$

$$\frac{\partial P_p^z}{\partial t} = -\alpha_p P_p^z - \beta_p Q_p^z + \delta_p E^z, \quad p = 1, \dots, P; \quad (4.16)$$

$$\frac{\partial Q_p^z}{\partial t} = -\alpha_p Q_p^z + \beta_p P_p^z - \gamma_p E^z, \quad p = 1, \dots, P.$$

$$\left. \begin{aligned} \frac{\partial P_l}{\partial t} &= A_l^{x,r} H^y + B_l^{x,r} P_l - B_l^{x,i} Q_l \\ \frac{\partial Q_l}{\partial t} &= A_l^{x,i} H^y + B_l^{x,i} P_l + B_l^{x,r} Q_l \end{aligned} \right\} \quad l = 1, \dots, L \quad (4.17)$$

We assign to Au -part the following terms:

- in equation (4.12): $\frac{1}{\varepsilon_\infty} \sum_{p=1}^P \alpha_p P_p^x + \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \beta_p Q_p^x - \frac{1}{\varepsilon_\infty} \sum_{p=1}^P \delta_p E^x$

- in equation (4.13): $-\frac{1}{\sqrt{\mu\epsilon_0\epsilon_\infty}} \sum_{l=1}^L P_l$
- in equation (4.14): $\frac{1}{\epsilon} \frac{\partial H^y}{\partial x} + \frac{1}{\epsilon_\infty} \sum_{p=1}^P \alpha_p P_p^z + \frac{1}{\epsilon_\infty} \sum_{p=1}^P \beta_p Q_p^z - \frac{1}{\epsilon_\infty} \sum_{p=1}^P \delta_p E^z,$
 $-\alpha_p P_p^x - \beta_p Q_p^x + \delta_p E^x, \quad p = 1, \dots, P;$
- in equation (4.15):
 $-\alpha_p Q_p^x + \beta_p P_p^x - \gamma_p E^x, \quad p = 1, \dots, P;$
 $-\alpha_p P_p^z - \beta_p Q_p^z + \delta_p E^z, \quad p = 1, \dots, P;$
- in equation (4.16):
 $-\alpha_p Q_p^z + \beta_p P_p^z - \gamma_p E^z, \quad p = 1, \dots, P.$
- in equation (4.17):
 $A_l^{x,r} H^y + B_l^{x,r} P_l - B_l^{x,i} Q_l, \quad l = 1, \dots, L;$
 $A_l^{x,i} H^y + B_l^{x,i} P_l + B_l^{x,r} Q_l, \quad l = 1, \dots, L.$

We assign to Bu -part the following terms:

- in equation (4.12): $-\frac{1}{\epsilon} \frac{\partial H^y}{\partial z}$
- in equation (4.13): $\frac{-\nu}{\sqrt{\mu\epsilon_0\epsilon_\infty}} \frac{\partial H^y}{\partial z}$
- in equation (4.14): nothing
- in equation (4.15): nothing
- in equation (4.16): nothing
- in equation (4.17): nothing.

References

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