

A PML method for signal-propagation problems in axon

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Abstract

This work is focused on the modelling of signal propagations in myelinated axons to characterize the functions of the myelin sheath in the neural structure. Based on reasonable assumptions on the medium properties, we derive a two-dimensional neural-signaling model in cylindrical coordinates from the time-harmonic Maxwell's equations. The well-posedness of model is established upon Dirichlet boundary conditions at the two ends of the neural structure and the radiative condition in the radial direction of the structure. Using the perfectly matched layer (PML) method, we truncate the unbounded background medium and propose an approximate problem on the truncated domain. The well-posedness of the PML problem and the exponential convergence of the approximate solution to the exact solution are established. Numerical experiments based on finite element discretization are presented to demonstrate the theoretical results and the efficiency of our methods to simulate the signal propagation in axons.

Keywords: Neural signal transmission, myelin sheath, Maxwell equation, perfectly-matched-layer

1 Introduction

The problem of the signal transmission in neural system is one of the most fundamental and important issues in neuroscience. Axons are the primary transmission lines of the nervous system and can be characterized into two types: myelinated and unmyelinated axons. It is studied in [16] that generation of new myelin is important for learning motor skills. For the myelinated axons, the myelin sheath is a layer of membrane wrapped around the axons and gaps in the myelin sheath, known as nodes of Ranvier, occur at evenly spaced intervals. It is understood that the functions of the myelin sheath and nodes of Ranvier are to insulate and cause the saltatory conduction of the action potential. However, it seems extremely difficult to experimentally observe the signal propagation in axon and quantitatively or qualitatively describe the effects of myelin sheath and nodes of Ranvier. Therefore, it has become more and more important to derive and investigate efficient mathematical and physical models to numerically simulate the transmission of signal in axon.

In open literature, the transmission of signals in axon is commonly treated by an equivalent circuit, see for example [10]. However, the model of an equivalent circuit, wherein frequencies in the kHz range is considered, is not consistent with the fact that biological macromolecules usually exhibit collective vibrations in the electromagnetic field in the infrared to terahertz (THz) spectral range [13, 17, 20] and furthermore, the roles of myelin features remain poorly understood. Recently, a novel dielectric waveguide model is proposed in [14] to explain the mechanism of infrared and terahertz neurotransmission through myelinated nerves. It is experimentally demonstrated in [14] that, at a certain THz/infrared frequency region, myelin exhibits a significantly higher refractive index than axons which supports the hypothesis that the myelin sheath serves as a dielectric waveguide. Then based on an electromagnetic waveguide model, the explicit waveguide modes can be calculated by assuming that an infinite axon is completely wrapped by the myelin sheath without any node of Ranvier. But this analytic method is not applicable for the case of finite myelinated axon with nodes of Ranvier, for which, only a schematic illustration has been provided. The numerical simulation of analogous waveguide models for myelinated axon has also been considered in [21, 22].

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However, these results still can not effectively characterize the functions of myelin sheath, and moreover, there is no mathematical and numerical analysis, for example, the well-posedness and convergence, for the considered model and associated numerical solver.

Inspired by [14, 21, 22], this paper devotes to proposing a novel waveguide problem of the electromagnetic waves to model the signal transmission in myelinated axon and providing solid mathematical analysis and numerical demonstration for the deduced model, for which the corresponding numerical analysis is left for future works. As shown in Figure 1(a), the signal propagation in the integrated neuron is quite complicated. Given an electromagnetic signal at one end of the axon, the propagation interested in this work is only restricted to the axon region as well as the myelin sheath. As shown in Figure 1(b) in cylindrical coordinates, let D_1 , D_2 denote the domain of axon and myelin sheath, respectively. Note that the skin depth is much larger than the neurological scale. Thus, exterior to the myelinated axon, an infinite domain D^c of fluid is assumed, see Figure 1(b). In addition, the cross section of myelinated axon can be viewed as a concentric structure. Then from the classical Maxwell's equations and assuming the wave fields to be always perpendicular to the direction of propagation (i.e., the length direction of axon) and independent of the angle variable, new time-harmonic TM and TE models in cylindrical coordinates, are introduced and appropriate boundary conditions are imposed at the end of axon Γ_{left} , Γ_{right} for approximation. Given an incident field on Γ_{left} , a zero mixed Dirichlet and Neumann boundary condition on Γ_{right} is considered. The discussion of the corresponding time-dependent model remains individually interesting and is left for future works.

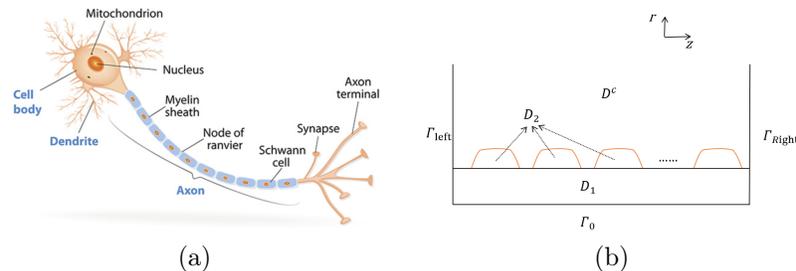


Figure 1: Left: a cartoon representation of a neuron with a myelinated axon [1]. Right: geometric settings for the mathematical model.

Then the main theoretical part of this work lies in proving the well-posedness of the derived electromagnetic problem and the convergence of the solution to an approximate problem resulting from the perfectly-matched-layer (PML) truncation. In both mathematical and engineering communities, related wave propagation problems in electromagnetics, as well as in acoustics and elastodynamics, have been extensively investigated [7, 12, 18], wherein the Dirichlet-to-Neumann (DtN) map [8, 9, 11] or the PML stretching [2, 4, 6] is commonly utilized to truncate the unbounded domain. For the newly derived electromagnetic problem, an exact DtN map and appropriate Sobolev spaces in cylindrical coordinates are introduced to prove the well-posedness of the corresponding variational problem as well as an inf-sup condition related to the weak formulation. The DtN truncated problem can be used for the numerical implementation, however, the DtN map is defined as an infinite series which is nonlocal and requires to be truncated into a finite sum in practical computation. Compared with the DtN technique, The PML method, first proposed by Bérenger for solving the time-dependent Maxwell equations [3] and considered in [21, 22] for different models of nerve signal propagation, takes advantages in numerical implementation and provides a viable alternative for solving the considered problem. Relying on the error estimate between the exact DtN map and the PML equivalent DtN map, the well-posedness and exponential convergence of the solution to the PML truncated problem are established. Then numerical experiments are reported to both verify our theoretical results and provide efficient simulation results to characterize the signal transmission phenomenon in axon, especially, the existence of myelin sheath can gather the electromagnetic wave to propagate mainly in myelin sheath.

The remainder of this paper is organized as follows. Section 2 proposes an electromagnetic scattering problem in cylindrical coordinates to model the signal transmission in myelinated axon. Then the well-posedness of the problem in appropriate Sobolev space is investigated in Section 3 by utilizing an exact DtN map to reduce the original problem onto a bounded domain. The PML stretching technique is introduced in Section 4 and then the well-posedness of the PML truncated problem, as well as the exponential convergence of the solutions with respect to PML parameters, is proved. Numerical experiments are presented in Section 5 to demonstrate the accuracy of the numerical solver and the efficiency of the mathematical model, especially, to provide an intuitive numerical description for the signal transmission in myelinated axon.

2 Mathematical model

Following the discussion in introduction, as shown in Figure 1(b), this section devotes to deriving a new electromagnetic problem in cylindrical coordinates to model the signal propagation in axon.

2.1 Governing equations

We begin with the Maxwell's equations given by

$$-i\omega\mu\mathbf{H} + \mathbf{curl}\mathbf{E} = \mathbf{0}, \quad (2.1a)$$

$$i\omega\varepsilon\mathbf{E} + \mathbf{curl}\mathbf{H} = \sigma\mathbf{E}. \quad (2.1b)$$

Here, ε , μ and σ denote the electric permittivity, the magnetic permeability, and the electric conductivity, respectively and we assume that μ is a positive constant and ε, σ are nonnegative and piece-wise constant. Compared with the axon, the electric conductivity in myelin sheath and water can be ignored and thus, $\sigma = 0$ in D_2 and D^c . By eliminating \mathbf{H} or \mathbf{E} , the second-order equation

$$\mathbf{curl}\mathbf{curl}\mathbf{E} - (k^2 + i\omega\mu\sigma)\mathbf{E} = \mathbf{0}, \quad (2.2)$$

holds for the electric field \mathbf{E} where $k = \omega\sqrt{\varepsilon\mu}$, and the second-order equation

$$\mathbf{curl}[(k^2 + i\omega\mu\sigma)^{-1}\mathbf{curl}\mathbf{H}] - \mathbf{H} = \mathbf{0}. \quad (2.3)$$

holds for the magnetic field \mathbf{H} .

Since axons usually maintain a constant radius, we next consider the Maxwell's equations in cylindrical coordinates and write

$$\mathbf{E} = E_r\hat{r} + r^{-1}E_\theta\hat{\theta} + E_z\hat{z}, \quad \mathbf{H} = H_r\hat{r} + r^{-1}H_\theta\hat{\theta} + H_z\hat{z}, \quad (2.4)$$

where \hat{r} , $\hat{\theta}$, \hat{z} are the unit vectors in the positive r -, θ -, and z -directions, respectively. Then for the TM mode, (2.2) is reduced to

$$r\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial E_\theta}{\partial r}\right) + \frac{\partial^2 E_\theta}{\partial z^2} + (k^2 + i\omega\mu\sigma)E_\theta = 0. \quad (2.5)$$

Similarly, for the TE mode, we can derive from (2.3) that

$$r\frac{\partial}{\partial r}\left(\frac{1}{(k^2 + i\omega\mu\sigma)r}\frac{\partial H_\theta}{\partial r}\right) + \frac{\partial}{\partial z}\left(\frac{1}{k^2 + i\omega\mu\sigma}\frac{\partial H_\theta}{\partial z}\right) + H_\theta = 0. \quad (2.6)$$

Denote $\Omega = (0, +\infty) \times (0, Z)$. Then in D^c where $\sigma = 0$, both (2.5) and (2.6) take a simplified form as follows:

$$r\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial u}{\partial r}\right) + \frac{\partial^2 u}{\partial z^2} + k^2u = 0, \quad u = E_\theta \text{ or } H_\theta. \quad (2.7)$$

2.2 Boundary and radiation conditions

To complete the modeling of signal propagation in axon, we impose the boundary conditions

$$\begin{cases} u(r, 0) = u_0(r) & \text{on } \Gamma_{\text{left}}, \\ \frac{\partial u}{\partial z}(r, Z) = u_N(r) & \text{on } \Gamma_{\text{right}}^1 := \Gamma_{\text{right}} \cap \partial D_1, \\ u(r, Z) = u_1(r) & \text{on } \Gamma_{\text{right}}^c := \Gamma_{\text{right}} \cap \partial D^c, \end{cases} \quad (2.8)$$

for $u = E_\theta$ or $u = H_\theta$ on Γ_{left} and Γ_{right} , and $u_0(r), u_1(r)$ are compactly supported, i.e., there exists some $R > 0$ such that for $r > R$, $u_0(r) = u_1(r) = 0$. On the other hand, since both \mathbf{E} and \mathbf{H} are bounded at $r = 0$, (2.4) indicates that on Γ_0 ,

$$\lim_{r \rightarrow 0} r^{-1}u = 0 \quad \forall z \in [0, Z]. \quad (2.9)$$

Moreover, it is necessary to force appropriate radiation condition for u as $r \rightarrow \infty$. The commonly used Silver-Müller radiation conditions for the electromagnetic fields \mathbf{E}, \mathbf{H} are given by

$$\lim_{|\mathbf{x}| \rightarrow \infty} |\mathbf{x}| |\mathbf{curl}\mathbf{E} \times \hat{\mathbf{x}} - i k \mathbf{E}| = 0, \quad \lim_{|\mathbf{x}| \rightarrow \infty} |\mathbf{x}| |\mathbf{curl}\mathbf{H} \times \hat{\mathbf{x}} - i k \mathbf{H}| = 0.$$

Then we assume that $u = E_\theta$ or H_θ admits the radiation condition as

$$\lim_{r \rightarrow \infty} \left| \frac{\partial u}{\partial r} - iku \right| = 0. \quad (2.10)$$

3 The well-posedness analysis

This section devotes to studying the well-posedness of the electromagnetic model derived in Section 2 through the variational approach. For simplicity, we only consider the problem of TM mode which consists of the equation (2.5), the boundary conditions (2.8)-(2.9) and the radiation condition (2.10). The results for the problem of TE mode can be carried out analogously and thus is omitted here. For the convenience of the following investigations, we denote by $\Omega_r = \{(\xi, \eta) : 0 < \xi < r, 0 < \eta < Z\}$ a truncated domain and denote the boundary $\Gamma_r = \{(r, z) : 0 < z < Z\}$, $\Sigma_r = \partial\Omega_r \setminus (\Gamma_r \cup \Gamma_0 \cup \Gamma_{\text{right}}^1)$. Denote $D_r^c = \Omega_r \setminus \overline{D_1 \cup D_2}$. Let $R > 0$ be large enough such that $\text{supp}(u_0) \cup \text{supp}(u_1) \subset [0, R]$ and $\text{supp}(\sigma) \subset \Omega_R$.

3.1 Sobolev spaces on the truncated domain

First we introduce some Sobolev spaces and their trace spaces in cylindrical coordinates. We define the space U_R equipped with a weighted L^2 -norm as

$$U_R = \{v \in L^2(\Omega_R) : \|v\|_{U_R} < \infty\}, \quad \|v\|_{U_R}^2 = \int_{\Omega_R} |u|^2 r^{-1} dr dz.$$

The subspaces V_R and $V_{R,0}$ equipped with a weighted H^1 -norm are defined as

$$V_R = \{v \in H^1(\Omega_R) : \|v\|_{V_R} < \infty, \lim_{r \rightarrow 0} r^{-1}v = 0\}, \quad V_{R,0} = \{v \in V_R : v|_{\Sigma_R} = 0\},$$

and

$$\|v\|_{V_R}^2 = \int_{\Omega_R} \left(\left| \frac{\partial u}{\partial r} \right|^2 + \left| \frac{\partial u}{\partial z} \right|^2 \right) r^{-1} dr dz + k^2 \|v\|_{U_R}^2.$$

Lemma 3.1. *The injection from V_R into U_R is compact.*

Proof. Let $\{v_n\}_{n=1}^\infty \subset V_R$ be a bounded sequence. The compact injection $V_R \hookrightarrow L^2(\Omega_R)$ implies that there exists a subsequence $\{v_{n_k}\}$ which is convergent in $L^2(\Omega_R)$ and thus, $\|e_{ij}\|_{L^2(\Omega_R)} \rightarrow 0$ as $i, j \rightarrow \infty$ where $e_{ij} := v_{n_i} - v_{n_j}$. Since e_{ij} vanishes on Γ_0 for all i and j , we deduce that

$$\begin{aligned} \int_{\Omega_R} \frac{1}{r} |e_{ij}(r, z)|^2 dr dz &= \int_{\Omega_R} \frac{1}{r} \bar{e}_{ij}(r, z) \left[\int_0^r \frac{\partial e_{ij}}{\partial t}(t, z) dt \right] dr dz \\ &\leq \|e_{ij}\|_{L^2(\Omega_R)} \left[\int_{\Omega_R} \frac{1}{r^2} \left| \int_0^r \frac{\partial e_{ij}}{\partial t}(t, z) dt \right|^2 dr dz \right]^{1/2} \\ &\leq \|e_{ij}\|_{L^2(\Omega_R)} \left[\int_{\Omega_R} \frac{1}{r} \int_0^r \left| \frac{\partial e_{ij}}{\partial t}(t, z) \right|^2 dt dr dz \right]^{1/2} \\ &\leq \|e_{ij}\|_{L^2(\Omega_R)} \left[\int_{\Omega_R} \int_0^R \frac{1}{t} \left| \frac{\partial e_{ij}}{\partial t}(t, z) \right|^2 dt dr dz \right]^{1/2} \\ &= R^{1/2} \|e_{ij}\|_{L^2(\Omega_R)} \|e_{ij}\|_{V_R}. \end{aligned}$$

Hence, $\{v_{n_k}\}$ is a Cauchy sequence under the norm $\|\cdot\|_{U_R}$. It is easy to see that U_R is a Banach space. Therefore, the subsequence $\{v_{n_k}\}$ is convergent in U_R which means that V_R is compactly embedded into U_R . \square

Now we study the Sobolev spaces on Γ_R . For any $v \in L^2(\Gamma_R)$, we can write it into a Fourier series $v = \sum_{m=0}^\infty [v_{1,m} \cos(m\pi z/Z) + v_{2,m} \sin(m\pi z/Z)]$. An equivalent norm on $L^2(\Gamma_R)$ is defined by the Parseval identity

$$\|v\|_{L^2(\Gamma_R)}^2 = \frac{Z}{2} \sum_{m=0}^\infty (|v_{1,m}|^2 + |v_{2,m}|^2).$$

Similarly, the norm on $H^{1/2}(\Gamma_R)$ is defined as

$$\|v\|_{H^{1/2}(\Gamma_R)}^2 = \sum_{m=0}^\infty m (|v_{1,m}|^2 + |v_{2,m}|^2).$$

Let $H_0^{1/2}(\Gamma_R)$ denote the closure of $C_0^\infty(\Gamma_R)$ in $H^{1/2}(\Gamma_R)$, namely,

$$H_0^{1/2}(\Gamma_R) := \overline{C_0^\infty(\Gamma_R)}^{\|\cdot\|_{H^{1/2}(\Gamma_R)}}. \quad (3.1)$$

It is easy to see that $H_0^{1/2}(\Gamma_R)$ is the trace space of $V_{R,0}$ on Γ_R . The dual space of $H_0^{1/2}(\Gamma_R)$ is denoted by $H^{-1/2}(\Gamma_R) := [H_0^{1/2}(\Gamma_R)]'$. Any $w \in H_0^{1/2}(\Gamma_R)$ admits a Fourier expansion $w = \sum_{m=1}^\infty w_m \sin(m\pi z/Z)$. The equivalent norms on $H_0^{1/2}(\Gamma_R)$ and $H^{-1/2}(\Gamma_R)$ are, respectively, defined as

$$\|w\|_{H_0^{1/2}(\Gamma_R)}^2 = \sum_{m=1}^\infty m |w_m|^2, \quad \|w\|_{H^{-1/2}(\Gamma_R)}^2 = \sum_{m=1}^\infty m^{-1} |w_m|^2.$$

3.2 Dirichlet-to-Neumann (DtN) map and truncated problem

Since $u(r, 0) = u(r, Z) = 0$ for $r \geq R$, we can write u into a Fourier series $u(r, z) = \sum_{m=1}^\infty u_m(r) \sin(m\pi z/Z)$ for $r \geq R, 0 \leq z \leq Z$. Substituting the series into (2.7), we get an ordinary differential equation

$$u_m''(r) - r^{-1}u_m'(r) + k_m^2 u_m(r) = 0, \quad k_m = \begin{cases} \sqrt{k^2 - m^2\pi^2/Z^2} & \text{if } k > m\pi/Z, \\ \mathbf{i}\sqrt{m^2\pi^2/Z^2 - k^2} & \text{otherwise.} \end{cases} \quad (3.2)$$

To eliminate resonance mode, we assume that $k \neq m\pi/Z$ for all $m \geq 1$. Using (2.10), the outgoing solution of (3.2) is given by

$$u_m(r) = a_m r H_1^{(1)}(k_m r), \quad (3.3)$$

where $H_1^{(1)}$ is the first order Hankel function of the first kind. It is easy to see that

$$\frac{\partial}{\partial r}(r^{-1}u) = r^{-2} \sum_{m=1}^\infty h(k_m r) u_m(r) \sin(m\pi z/Z), \quad h(t) := t H_1^{(1)'}(t) / H_1^{(1)}(t). \quad (3.4)$$

Remark 3.2. Since $|H_1^{(1)}(t)| \sim t^{-1/2}$ as $t \rightarrow +\infty$, equation (3.3) implies that $|u_m(r)|$ grows at the rate $r^{1/2}$ as $r \rightarrow +\infty$. In view of (2.4), it is $r^{-1}u$ that represents the angular component of \mathbf{E} or \mathbf{H} . Therefore, the growing rate of $u_m(r)$ is reasonable.

For any $\eta \in H_0^{1/2}(\Gamma_R)$ which admits a Fourier series $\eta = \sum_{m=1}^\infty \eta_m \sin(m\pi z/Z)$, we define a Dirichlet-to-Neumann (DtN) map $T : H_0^{1/2}(\Gamma_R) \rightarrow H^{-1/2}(\Gamma_R)$ by

$$T\eta = \frac{\partial}{\partial r}(r^{-1}v)|_{\Gamma_R},$$

where v is the solution of (2.7) in $\Omega_R^c = \Omega^c \setminus \overline{\Omega_R}$ satisfying the Dirichlet boundary conditions $v(R, z) = \eta$ for $0 \leq z \leq Z$ and $v(r, 0) = v(r, Z) = 0$ for $r \geq R$, and the radiation condition (2.10). Using (3.4), the DtN map can be expressed as

$$T\eta = \sum_{m=1}^\infty h(k_m R) \eta_m \sin(m\pi z/Z). \quad (3.5)$$

Utilizing the continuity of the fields crossing the boundary Γ_R , we can reformulate the model of TM mode on the truncated domain

$$r \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial u}{\partial r} \right) + \frac{\partial^2 u}{\partial z^2} + (k^2 + i\omega\mu\sigma)u = 0 \quad \text{in } \Omega_R, \quad (3.6a)$$

$$\lim_{r \rightarrow 0} r^{-1}u = 0 \quad \text{on } \Gamma_0, \quad (3.6b)$$

$$u = u_D \quad \text{on } \Sigma_R, \quad (3.6c)$$

$$\frac{\partial u}{\partial z} = u_N \quad \text{on } \Gamma_{\text{right}}^1, \quad (3.6d)$$

$$\frac{\partial}{\partial r}(r^{-1}u) = R^{-2}Tu \quad \text{on } \Gamma_R, \quad (3.6e)$$

where $u_D \in H^{1/2}(\Sigma_R)$ is defined as

$$u_D = u_0 \text{ on } \Gamma_{\text{left}}, \quad u_D = u_1 \text{ on } \Gamma_{\text{right}}^c.$$

Multiplying both sides of (3.6a) with v/r where $v \in V_{R,0}$, integrating the result on Ω_R and taking integration by part, we can obtain the corresponding variational problem of (3.6) as follows: find $u \in V_R$ such that $u = u_D$ on Σ_R and

$$a(u, v) = \int_{\Gamma_{\text{right}}^1} u_N \bar{v} dr \quad \forall v \in V_{R,0}, \quad (3.7)$$

where a is a sesquilinear form on $V_R \times V_R$ defined by

$$a(u, v) = \int_{\Omega_R} \left[\frac{\partial u}{\partial r} \frac{\partial \bar{v}}{\partial r} + \frac{\partial u}{\partial z} \frac{\partial \bar{v}}{\partial z} - (k^2 + \mathbf{i}\omega\mu\sigma)u\bar{v} \right] \frac{1}{r} dr dz - \frac{1}{R^2} \langle Tu + u, v \rangle_{\Gamma_R}. \quad (3.8)$$

Here $\langle \xi, v \rangle_{\Gamma_R} := \int_{\Gamma_R} \xi \bar{v} dz$ stands for the duality product if $\xi \in H^{-1/2}(\Gamma_R)$ and $v \in H_0^{1/2}(\Gamma_R)$ or the inner product if $\xi, v \in L^2(\Gamma_R)$.

3.3 The well-posedness of problem (3.7)

In this subsection, we shall prove the inf-sup condition for the sesquilinear form a and establish the well-posedness of problem (3.7). For any $v, w \in H_0^{1/2}(\Gamma_R)$, we always write $v = \sum_{m=1}^{\infty} v_m \sin(m\pi z/Z)$ and $w = \sum_{m=1}^{\infty} w_m \sin(m\pi z/Z)$. First we prove some useful results of the DtN map.

Lemma 3.3. $\text{Im}\langle Tv, v \rangle_{\Gamma_R} \geq 0$ for any $v \in H_0^{1/2}(\Gamma_R)$ and $\text{Im}\langle Tv, v \rangle_{\Gamma_R} = 0$ implies $v \in \text{Span}\{\sin(m\pi z/Z) : m > kZ/\pi\}$.

Proof. It follows from (3.5) that $\text{Im}\langle Tv, v \rangle_{\Gamma_R} = \frac{Z}{2} \sum_{m=1}^{\infty} \text{Im}[h(k_m R)] |v_m|^2$ for any $v \in H_0^{1/2}(\Gamma_R)$. For $k > m\pi/Z$, we have $k_m > 0$. Recalling that for $t > 0, l \in \mathbb{Z}$, $H_l^{(1)}(t) = J_l(t) + \mathbf{i}Y_l(t)$ and $J_l(t)Y_{l-1}(t) - J_{l-1}(t)Y_l(t) = 2/(\pi t)$, we have

$$H_{l-1}^{(1)}(t) \overline{H_l^{(1)}(t)} = J_{l-1}(t)J_l(t) + Y_{l-1}(t)Y_l(t) + 2\mathbf{i}/(\pi t) \quad \forall t > 0, l \in \mathbb{Z}.$$

Therefore, from the relation $tH_1^{(1)'}(t) = tH_0^{(1)}(t) - H_1^{(1)}(t)$, we know

$$\text{Im}[h(k_m R)] = \left| H_1^{(1)}(t) \right|^{-2} \text{Im} \left[tH_0^{(1)}(t) \overline{H_1^{(1)}(t)} \right] = \frac{2}{\pi} \left| H_1^{(1)}(k_m R) \right|^{-2} > 0. \quad (3.9)$$

For $k < m\pi/Z$, we recall the modified Bessel functions K_l which satisfy

$$H_l^{(1)}(\mathbf{i}t) = \frac{2}{\pi} e^{-(l+1)\pi/2\mathbf{i}} K_l(t), \quad t > 0. \quad (3.10)$$

Since $K_l(t)$ are real for all l and $t > 0$, from (3.4) and (3.10), we easily know that $\text{Im}[h(k_m R)] = 0$. The proof is complete. \square

Lemma 3.4. *There exists a constant $C > 0$ depending only on k, R , and Z such that*

$$\|Tv\|_{H^{-1/2}(\Gamma_R)} \leq C \|v\|_{H^{1/2}(\Gamma_R)} \quad \forall v \in H_0^{1/2}(\Gamma_R).$$

Proof. Note that for $1 \leq m < kZ/\pi$, $k_m > 0$. We know from [15, (3.17)] that

$$\frac{4k_m^2 R^2}{4k_m^2 R^2 + 3} \leq -\text{Re} h(k_m R) \leq \frac{1}{2} + \frac{9}{16k_m^2 R^2}. \quad (3.11)$$

Then (3.9) and (3.11) yield that there exists a constant $C > 0$ depending only on k such that $|h(k_m R)| \leq C$. For $m > kZ/\pi$, from (3.10), the positivity of $K_m(t)$ for all $m \geq 0, t > 0$ and [19, eq. (10.37.1)], we have

$$-h(k_m R) = 1 + |k_m| R \frac{K_0(|k_m| R)}{K_1(|k_m| R)} \leq 1 + |k_m| R \leq 1 + m\pi R/Z.$$

For any $v, w \in H_0^{1/2}(\Gamma_R)$, we have

$$\begin{aligned} |\langle Tv, w \rangle_{\Gamma_R}| &= \frac{Z}{2} \sum_{m=1}^{\infty} |h(k_m R) v_m \overline{w_m}| && \leq C \sum_{m=1}^{\infty} m |v_m \overline{w_m}| \\ &&& \leq C \|v\|_{H^{1/2}(\Gamma_R)} \|w\|_{H^{1/2}(\Gamma_R)}. \end{aligned}$$

This leads to

$$\|Tv\|_{H^{-1/2}(\Gamma_R)} = \sup_{w \in H_0^{1/2}(\Gamma_R)} \frac{|\langle Tv, w \rangle_{\Gamma_R}|}{\|w\|_{H^{1/2}(\Gamma_R)}} \leq C \|v\|_{H^{1/2}(\Gamma_R)}.$$

The proof is finished. \square

The proof of Lemma 3.4 also indicates the following useful result.

Lemma 3.5. *It holds that $-\operatorname{Re}\langle Tv, v \rangle_{\Gamma_R} \geq 0$ for all $v \in H_0^{1/2}(\Gamma_R)$.*

The uniqueness of the variational problem (3.7) is given in the following lemma.

Lemma 3.6. *The variational problem (3.7) has at most one solution.*

Proof. Since (3.7) is a linear problem, it suffices to show that $u_D = u_N = 0$ implies $u \equiv 0$. Now we suppose $u \in V_{R,0}$ and take $v = u$ in (3.7). The imaginary part of the equation shows

$$\omega\mu \int_{\Omega_R} \sigma |u|^2 r^{-1} dr dz + R^{-2} \operatorname{Im}\langle Tu, u \rangle_{\Gamma_R} = 0.$$

From Lemma 3.3, we infer that $u \equiv 0$ in D_1 . From (2.7), we have

$$r \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial u}{\partial r} \right) + \frac{\partial^2 u}{\partial z^2} + k^2 u = 0 \quad \text{in } \Omega_R \setminus \overline{D_1}.$$

Since $u \equiv 0$ in D_1 , we also have

$$r \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial u}{\partial r} \right) + \frac{\partial^2 u}{\partial z^2} + k^2 u = 0 \quad \text{in } \Omega_R. \quad (3.12)$$

Take a $\mathbf{p} \in \partial D_1$ and an open disk $B_\delta(\mathbf{p})$ with the radius δ and the center being \mathbf{p} . Assume $B_\delta(\mathbf{p}) \subset \Omega_R$ without loss of generality. There exists a constant depending on δ and k such that

$$\left| \frac{\partial^2 u}{\partial r^2} + \frac{\partial^2 u}{\partial z^2} \right| \leq C \left(\left| \frac{\partial u}{\partial r} \right| + |u| \right) \quad \text{a.e. in } B_\delta(\mathbf{p}).$$

Note that $u \equiv 0$ in $B_\delta(\mathbf{p}) \cap D_1$. By the unique continuation theory (see Lemma 4.15 in [18], page 93), we have $u \equiv 0$ in $B_\delta(\mathbf{p})$. Moreover, we can extend the arguments from $B_\delta(\mathbf{p})$ to Ω_R and end up with $u \equiv 0$ in Ω_R . \square

Now, we are ready to show the inf-sup condition for the sesquilinear form a and establish the well-posedness of problem (3.7).

Theorem 3.7. *There exists a unique solution to the variational problem (3.7). Moreover, the inf-sup condition*

$$\sup_{0 \neq v \in V_{R,0}} \frac{|a(w, v)|}{\|v\|_{V_R}} \geq C_{\inf} \|w\|_{V_R}, \quad \forall w \in V_{R,0},$$

holds where $C_{\inf} > 0$ is a constant depending only on k, R, Z and material parameters.

Proof. It suffices to prove that, for any $\ell \in V'_{R,0}$, there exists a unique solution $w \in V_{R,0}$ to the problem

$$a(w, v) = \ell(v) \quad \forall v \in V_{R,0}, \quad (3.13)$$

and that the solution satisfies $\|w\|_{V_R} \leq C \|\ell\|_{V'_{R,0}}$. To do this, we define another sesquilinear form a_+ on $V_R \times V_R$ as

$$a_+(u, v) = \int_{\Omega_R} \left[\frac{\partial u}{\partial r} \frac{\partial \bar{v}}{\partial r} + \frac{\partial u}{\partial z} \frac{\partial \bar{v}}{\partial z} + (k^2 - \mathbf{i}\omega\mu\sigma)u\bar{v} \right] \frac{1}{r} dr dz - \frac{1}{R^2} \langle Tu, v \rangle_{\Gamma_R}. \quad (3.14)$$

By Lemmas 3.3-3.5, there is a generic constant $C > 0$ depending only on k, R, Z and material parameters such that

$$|a_+(v, v)| \geq \operatorname{Re} a_+(v, v) \geq \|v\|_{V_R}^2, \quad |a_+(u, v)| \leq C \|u\|_{V_R} \|v\|_{V_R}. \quad (3.15)$$

Let $\mathcal{K}_0 : U_R \rightarrow V_{R,0}$ and $\mathcal{K}_1 : L^2(\Gamma_R) \rightarrow V_{R,0}$ be two operators defined as follows: for $w \in U_R$ and $\eta \in L^2(\Gamma_R)$, $\mathcal{K}_0 w$ and $\mathcal{K}_1 \eta$ are the unique solutions to the following two problems, respectively,

$$a_+(\mathcal{K}_0 w, v) = 2k^2 \int_{\Omega_R} w \bar{v} \frac{1}{r} dr dz, \quad a_+(\mathcal{K}_1 \eta, v) = R^{-2} \langle \eta, v \rangle_{\Gamma_R} \quad \forall v \in V_{R,0}. \quad (3.16)$$

Then (3.15) together with Lax-Milgram theorem implies that \mathcal{K}_0 and \mathcal{K}_1 are continuous operators, namely,

$$\|\mathcal{K}_0 w\|_{V_R} \leq C \|w\|_{U_R}, \quad \|\mathcal{K}_1 \eta\|_{V_R} \leq C \|\eta\|_{L^2(\Gamma_R)}.$$

By Lemma 3.1 and the compact injection $H^{1/2}(\Gamma_R) \hookrightarrow L^2(\Gamma_R)$, both $\mathcal{K}_0 : V_{R,0} \rightarrow V_{R,0}$ and $\mathcal{K}_1 : H_0^{1/2}(\Gamma_R) \rightarrow V_{R,0}$ are compact operators.

Let γ_R denote the trace operator which maps $V_{R,0}$ onto $H_0^{1/2}(\Gamma_R)$ continuously. We can write problem (3.13) into an equivalent operator equation

$$w - (\mathcal{K}_0 + \mathcal{K}_1 \gamma_R) w = f, \quad (3.17)$$

where $f \in V_{R,0}$ is the unique solution to the problem

$$a_+(f, v) = \ell(v) \quad \forall v \in V_{R,0}.$$

Since $\mathcal{K}_0 + \mathcal{K}_1 \gamma_R : V_{R,0} \rightarrow V_{R,0}$ is a compact operator, (3.17) is a Fredholm equation of second kind. By Lemma 3.6 and Fredholm alternative theorem, we conclude that there exists a unique solution to the variational problem (3.13). Let \mathcal{I} denote the identity operator on $V_{R,0}$. The arbitrariness of $\ell \in V'_{R,0}$ shows that $(\mathcal{I} - \mathcal{K}_0 - \mathcal{K}_1 \gamma_R)^{-1}$ exists and is a continuous operator from $V_{R,0}$ to $V_{R,0}$. We end up with

$$\|w\|_{V_R} \leq C \|f\|_{V_R} \leq C \|\ell\|_{V'_{R,0}} = C \sup_{0 \neq v \in V_{R,0}} \frac{|a(w, v)|}{\|v\|_{V_R}}.$$

The proof is complete. \square

Remark 3.8. *In this section, we establish the well-posedness for the derived electromagnetic model by introducing the exact DtN map to truncate the unbounded domain. Incorporating with the finite element method (FEM), which is called DtN-FEM, the variational problem (3.7) can be used for the numerical simulation. Noting that the discretization of the sesquilinear form $\langle Tu, v \rangle_{\Gamma_R}$ is a nonlocal integral, in the rest of this work we utilize an alternative way, the PML method, to truncate the unbounded domain Ω^c and study the convergence of this method. The analysis and application of DtN-FEM, including the truncation of the infinite series in the DtN map and adaptivity, are left for future works.*

4 The truncated PML problem and convergence study

Besides the DtN map discussed in Section 3, this section proposes an approximate problem applying the PML truncation strategy. Suppose $\rho \geq 2R$ and let $\Omega_\rho := \{0 < r < \rho, 0 < z < Z\}$ be the domain in which the truncated PML problem is formulated. Denote $\Omega_{\text{pml}} := \Omega_\rho \setminus \bar{\Omega}_R$ the PML region with $d = \rho - R$ being the thickness of Ω_{pml} . To derive the truncated PML problem, we introduce the following complex stretching of radial coordinate. Define

$$\tilde{r} = F(r) := r + (1 + \mathbf{i})\chi(r), \quad \chi(r) = \begin{cases} 0 & \text{if } r \leq R, \\ \chi_0(r - R)^2 & \text{if } r > R, \end{cases} \quad (4.1)$$

where $\chi_0 > 0$ is a constant. Clearly, χ is C^1 -smooth in $(0, +\infty)$. Denote

$$\alpha(r) = F'(r) = 1 + (1 + \mathbf{i})\chi'(r), \quad \beta(r) = \tilde{r}/r = 1 + (1 + \mathbf{i})\chi(r)/r. \quad (4.2)$$

We have already assumed that $k \neq m\pi/Z$ for all $m \geq 1$. Without loss of generality, we additionally assume

$$\kappa\chi_0 R \geq 1, \quad \kappa := \min_{m \geq 1} |k_m|. \quad (4.3)$$

4.1 The approximate problem

Note from (3.3) that, for $r \geq R$, the exact solution to problem (3.6) can be represented as

$$u(r, z) = r \sum_{m=1}^{\infty} a_m H_1^{(1)}(k_m r) \sin(m\pi z/Z) \quad \forall r \geq R. \quad (4.4)$$

With this explicit representation, we can define the analytic continuation of u from the real variable r to the complex variable \tilde{r} by

$$u(\tilde{r}, z) = \tilde{r} \sum_{m=1}^{\infty} a_m H_1^{(1)}(k_m \tilde{r}) \sin(m\pi z/Z) \quad \forall r \geq R. \quad (4.5)$$

Then by the chain rule, it is easy to see that $\tilde{u}(r, z) := u(\tilde{r}, z)$ satisfies the modified equation

$$\frac{r\beta}{\alpha} \frac{\partial}{\partial r} \left(\frac{1}{r\alpha\beta} \frac{\partial \tilde{u}}{\partial r} \right) + \frac{\partial^2 \tilde{u}}{\partial z^2} + (k^2 + i\omega\mu\sigma)\tilde{u} = 0 \quad \text{in } \Omega. \quad (4.6)$$

To truncate the unbounded domain Ω , it is reasonable to impose the Dirichlet boundary condition $\hat{u} = 0$ on Γ_ρ regarding to the exponential decay of the Hankel functions with a complex argument. Hence, the approximate problem to (3.6) is proposed as follows

$$\frac{r\beta}{\alpha} \frac{\partial}{\partial r} \left(\frac{1}{r\alpha\beta} \frac{\partial \hat{u}}{\partial r} \right) + \frac{\partial^2 \hat{u}}{\partial z^2} + (k^2 + i\omega\mu\sigma)\hat{u} = 0 \quad \text{in } \Omega_\rho, \quad (4.7a)$$

$$\lim_{r \rightarrow 0} r^{-1} \hat{u} = 0 \quad \text{on } \Gamma_0, \quad (4.7b)$$

$$\hat{u} = u_D \quad \text{on } \Sigma_\rho, \quad \hat{u} = 0 \quad \text{on } \Gamma_\rho, \quad (4.7c)$$

$$\frac{\partial \hat{u}}{\partial z} = u_N \quad \text{on } \Gamma_{\text{right}}^1. \quad (4.7d)$$

Letting the spaces $V_\rho, V_{\rho,0}$, as well as the equipped norms, be defined analogous to $V_R, V_{R,0}$, respectively, by replacing the domain Ω_R by Ω_ρ and denote $V_\rho^0 := \{v \in V_{\rho,0} : v|_{\Gamma_\rho} = 0\}$. Then the weak formulation of the problem (4.7) reads: find $\hat{u} \in V_\rho$ such that $\hat{u} = u_D$ on Σ_ρ and

$$a_\rho(\hat{u}, v) = \int_{\Gamma_{\text{right}}^1} u_N \bar{v} dr \quad \forall v \in V_\rho^0, \quad (4.8)$$

where

$$a_\rho(\hat{u}, v) := \int_{\Omega_\rho} \frac{1}{r\beta} \left(\frac{1}{\alpha} \frac{\partial \hat{u}}{\partial r} \frac{\partial \bar{v}}{\partial r} + \alpha \frac{\partial \hat{u}}{\partial z} \frac{\partial \bar{v}}{\partial z} - \alpha(k^2 + i\omega\mu\sigma)\hat{u}\bar{v} \right) dr dz.$$

The purpose of the remaining parts of this section is to study the well-posedness of the approximate problem (4.7) and its convergence, i.e., the error estimate between the exact solution u of problem (3.6) and the approximate solution \hat{u} of problem (4.7). Since problem (3.6) is defined on Ω_R , we next reformulate (4.7) into a problem on Ω_R utilizing the DtN map strategy. Let $\hat{T} : H_0^{1/2}(\Gamma_R) \rightarrow H^{-1/2}(\Gamma_R)$ be a DtN map defined as, for any $\eta \in H_0^{1/2}(\Gamma_R)$,

$$\hat{T}\eta := R^2 \frac{\partial}{\partial r} (r^{-1}w) \Big|_{\Gamma_R}, \quad (4.9)$$

where w is the solution to the Dirichlet problem in the PML

$$\frac{r\beta}{\alpha} \frac{\partial}{\partial r} \left(\frac{1}{r\alpha\beta} \frac{\partial w}{\partial r} \right) + \frac{\partial^2 w}{\partial z^2} + k^2 w = 0 \quad \text{in } \Omega_{\text{pml}}, \quad (4.10a)$$

$$w = \eta \quad \text{on } \Gamma_R, \quad (4.10b)$$

$$w = 0 \quad \text{on } \partial\Omega_{\text{pml}} \setminus \Gamma_R. \quad (4.10c)$$

The well-posedness of problem (4.10), which will be addressed in the next subsection, ensures that the DtN operator \hat{T} is well-defined. Then the continuity of the fields crossing the boundary Γ_R indicates that we can reformulate the problem (4.7) in Ω_R as follows:

$$r \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial \hat{u}}{\partial r} \right) + \frac{\partial^2 \hat{u}}{\partial z^2} + (k^2 + i\omega\mu\sigma)\hat{u} = 0 \quad \text{in } \Omega_R, \quad (4.11a)$$

$$\lim_{r \rightarrow 0} r^{-1} \hat{u} = 0 \quad \text{on } \Gamma_0, \quad (4.11b)$$

$$\hat{u} = u_D \quad \text{on } \Sigma_R, \quad (4.11c)$$

$$\frac{\partial \hat{u}}{\partial z} = u_N \quad \text{on } \Gamma_{\text{right}}^1, \quad (4.11d)$$

$$\frac{\partial}{\partial r} (r^{-1} \hat{u}) = R^{-2} \hat{T} \hat{u} \quad \text{on } \Gamma_R. \quad (4.11e)$$

This leads us to study the well-posedness of problem (4.11) and the error estimate between the exact solution u of problem (3.6) and the approximate solution \hat{u} of problem (4.11).

4.2 The well-posedness of problem (4.10)

To establish the well-posedness of problem (4.10), we use separation of variables and the Fourier expansions of w and η formulated as

$$w(r, z) = \sum_{m=1}^{\infty} w_m(r) \sin(m\pi z/Z), \quad \eta(z) = \sum_{m=1}^{\infty} \eta_m \sin(m\pi z/Z), \quad (4.12)$$

to reduce the problem (4.10) into a system of ordinary differential equations, for $m \geq 1$,

$$\frac{r\beta}{\alpha} \frac{\partial}{\partial r} \left(\frac{1}{r\alpha\beta} \frac{\partial w_m}{\partial r} \right) + k_m^2 w_m = 0 \quad \text{for } R < r < \rho, \quad (4.13a)$$

$$w_m(R) = \eta_m, \quad w_m(\rho) = 0. \quad (4.13b)$$

The variational formulation of (4.13) is given as follows: find $w_m \in H^1((R, \rho))$ which satisfies (4.13b) and

$$\mathcal{A}_m(w_m, v) := \int_R^\rho \frac{1}{r\beta} (\alpha^{-1} w_m' \bar{v}' - \alpha k_m^2 w_m \bar{v}) dr = 0 \quad \forall v \in H_0^1((R, \rho)). \quad (4.14)$$

We first prove the well-posedness of the problem (4.13) for each $m \geq 1$.

Lemma 4.1. *There exist two positive constants C_0, C_1 independent of m, χ_0 , and ρ such that, for any $v \in H_0^1((R, \rho))$,*

$$\text{Re } \mathcal{A}_m(v, v) \geq \int_R^\rho \xi |v'|^2 dr - C_0 k_m^2 \int_R^\rho \eta |v|^2 dr \quad \text{if } m > kZ/\pi, \quad (4.15)$$

$$\begin{aligned} & \text{Re } \mathcal{A}_m(v, v) - C_1 d^3 |\alpha(\rho)|^2 \text{Im } \mathcal{A}_m(v, v) \\ & \geq \frac{1}{2} \int_R^\rho \xi |v'|^2 dr + C_0 d^3 |\alpha(\rho)|^2 \int_R^\rho \eta \chi' |v|^2 dr \quad \text{if } m < kZ/\pi, \end{aligned} \quad (4.16)$$

where $\xi = (r + r\chi' + \chi)/|r\alpha\beta|^2$ and $\eta = (r + r\chi' + \chi + 2\chi\chi')/|r\beta|^2$. As a result, there exists a unique solution to the problem (4.13) for all $m \geq 1$.

Proof. Write $\xi_1 = (r\chi' + \chi + 2\chi\chi')/|r\alpha\beta|^2$ and $\eta_1 = (r\chi' - \chi)/|r\beta|^2$ for convenience. It is easy to see

$$\operatorname{Re} \mathcal{A}_m(v, v) = \int_R^\rho \left(\xi |v'|^2 - k_m^2 \eta |v|^2 \right), \quad (4.17)$$

$$\operatorname{Im} \mathcal{A}_m(v, v) = - \int_R^\rho \left(\xi_1 |v'|^2 + k_m^2 \eta_1 |v|^2 \right). \quad (4.18)$$

Since $k_m^2 = k^2 - m^2\pi^2/Z^2 < 0$ for $m > kZ/\pi$, (4.15) comes directly from (4.17). Next, we prove (4.16). Since $v(R) = 0$ and $\chi'(r) = 2\chi_0(r - R)$, we have

$$\begin{aligned} \int_R^\rho \eta |v|^2 dr &\leq \epsilon^{-1} \int_R^\rho \eta \chi' |v|^2 + \frac{\epsilon}{4} \int_R^\rho \frac{\eta(r)}{\chi'(r)} \left| \int_R^r v'(t) dt \right|^2 dr \\ &\leq \epsilon^{-1} \int_R^\rho \eta \chi' |v|^2 dr + C_2 \epsilon \chi_0 d^4 |\alpha(\rho)|^2 \int_R^\rho \xi |v'|^2 dr, \end{aligned} \quad (4.19)$$

where $\epsilon > 0$ is a constant to be specified and C_2 is a positive constant independent of m , χ_0 , and ρ . Inserting (4.19) into (4.17), we have

$$\operatorname{Re} \mathcal{A}_m(v, v) \geq \left[1 - C_2 \epsilon k_m^2 \chi_0 d^4 |\alpha(\rho)|^2 \right] \int_R^\rho \xi |v'|^2 dr - k_m^2 \epsilon^{-1} \int_R^\rho \eta \sigma' |v|^2 dr. \quad (4.20)$$

For (4.18), noting that there exists a positive constant C_3 independent of m , χ_0 , and ρ such that

$$\frac{\eta_1}{\eta \chi'} = \frac{r - \chi/\chi'}{r + r\chi' + \chi + 2\chi\chi'} \leq C_3,$$

we get

$$\operatorname{Im} \mathcal{A}_m(v, v) \leq -C_3 k_m^2 \int_R^\rho \eta \chi' |v|^2 dr. \quad (4.21)$$

Then combining (4.20) and (4.21) yields

$$\begin{aligned} \operatorname{Re} \mathcal{A}_m(v, v) - 2C_3^{-1} \epsilon^{-1} \operatorname{Im} \mathcal{A}_m(v, v) \\ \geq \left[1 - C_2 \epsilon k_m^2 \chi_0 d^4 |\alpha(\rho)|^2 \right] \int_R^\rho \xi |v'|^2 dr + \epsilon^{-1} k_m^2 \int_R^\rho \eta \chi' |v|^2 dr. \end{aligned} \quad (4.22)$$

Then choosing $\epsilon^{-1} = 2C_2 k_m^2 \chi_0 d^4 |\alpha(\rho)|^2$ gives (4.16).

Finally, the well-posedness of problem (4.13) for all $m \geq 1$ follows directly from the estimates (4.15)-(4.16). The proof is complete. \square

Now we are ready to get the the well-posedness of problem (4.10) which will further leads to a continuity estimate for the DtN map \hat{T} .

Theorem 4.2. *There exists a unique solution $w \in H^1(\Omega_{\text{pml}})$ to the problem (4.10). Moreover, there exists a constant $C > 0$ independent of χ_0 and ρ such that*

$$\|w\|_{H^1(\Omega_{\text{pml}})} \leq C d^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 \|\eta\|_{H^{1/2}(\Gamma_R)}.$$

Proof. There exists an extension $p \in H^1(\Omega_{2R} \setminus \bar{\Omega}_R)$ which satisfies $p = \eta$ on Γ_R , $p = 0$ on $\partial\Omega_{2R} \setminus \partial\Omega_R$, and

$$\|p\|_{H^1(\Omega_{2R} \setminus \bar{\Omega}_R)} \leq C \|\eta\|_{H^{1/2}(\Gamma_R)}, \quad (4.23)$$

where the constant C depends only on R and Z . Now we extend p by zero to $\Omega_\infty \setminus \bar{\Omega}_{2R}$ and designate the extension still by p . A weak formulation of (4.10) is to find $\hat{w} := w - p \in H_0^1(\Omega_{\text{pml}})$ such that

$$a_{\text{pml}}(\hat{w}, v) = -a_{\text{pml}}(p, v) \quad \forall v \in H_0^1(\Omega_{\text{pml}}),$$

where

$$a_{\text{pml}}(\hat{w}, v) := \int_{\Omega_{\text{pml}}} \frac{1}{r\beta} \left(\frac{1}{\alpha} \frac{\partial \hat{w}}{\partial r} \frac{\partial \bar{v}}{\partial r} + \alpha \frac{\partial \hat{w}}{\partial z} \frac{\partial \bar{v}}{\partial z} - \alpha k^2 \hat{w} \bar{v} \right).$$

Consider the Fourier series of \hat{w} and p with coefficients \hat{w}_m and p_m , respectively which satisfy $\hat{w}_m = w_m - p_m$. Define

$$\begin{aligned} W_1 &= \sum_{m < kZ/\pi} \hat{w}_m \sin(m\pi z/Z), & P_1 &= \sum_{m < kZ/\pi} p_m \sin(m\pi z/Z), \\ W_2 &= \sum_{m > kZ/\pi} \hat{w}_m \sin(m\pi z/Z), & P_2 &= \sum_{m > kZ/\pi} p_m \sin(m\pi z/Z). \end{aligned}$$

It is clear that $\hat{w} = W_1 + W_2$, $p = P_1 + P_2$, and

$$a_{\text{pml}}(W_1, W_1) = -a_{\text{pml}}(P_1, W_1), \quad a_{\text{pml}}(W_2, W_2) = -a_{\text{pml}}(P_2, W_2). \quad (4.24)$$

Let the function $\xi(r)$ and the constant C_1 be given in Lemma 4.1, and let the space $V(\Omega_{\text{pml}})$, as well as the equipped norm, be defined analogous to V_R . Using (4.16) and $\hat{w}_m(R) = 0$, we have

$$\begin{aligned} & \|W_1\|_{V(\Omega_{\text{pml}})}^2 \\ & \leq C \sum_{m < kZ/\pi} \left[\int_R^\rho \frac{1}{r} |\hat{w}'_m(r)|^2 dr + (k^2 + m^2\pi^2/Z^2) \int_R^\rho \frac{1}{r} \left| \int_R^r \hat{w}'_m(t) dt \right|^2 dr \right] \\ & \leq Cd^3 |\alpha(\rho)|^2 |\beta(\rho)|^2 \sum_{m < kZ/\pi} \int_R^\rho \xi(r) |\hat{w}'_m(r)|^2 dr \\ & \leq Cd^3 |\alpha(\rho)|^2 |\beta(\rho)|^2 \sum_{m < kZ/\pi} [\text{Re } \mathcal{A}_m(\hat{w}_m, \hat{w}_m) - C_1 d^3 |\alpha(\rho)|^2 \text{Im } \mathcal{A}_m(\hat{w}_m, \hat{w}_m)]. \end{aligned}$$

Using (4.24) and the relation $a_{\text{pml}}(W_1, W_1) = \frac{Z}{2} \sum_{m < kZ/\pi} \mathcal{A}_m(\hat{w}_m, \hat{w}_m)$, we deduce that

$$\|W_1\|_{V(\Omega_{\text{pml}})}^2 \leq Cd^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 |a_{\text{pml}}(P_1, W_1)|.$$

Since P_1 is only supported in $\Omega_{2R} \setminus \bar{\Omega}_R$, using (4.23) and Schwartz's inequality, we easily get

$$\|W_1\|_{V(\Omega_{\text{pml}})} \leq Cd^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 \|P_1\|_{V(\Omega_{2R} \setminus \bar{\Omega}_R)} \leq Cd^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 \|\eta\|_{H^{1/2}(\Gamma_R)}. \quad (4.25)$$

The estimate of W_2 is similar but easier. Since $k_m^2 < 0$ for $m > kZ/\pi$, we have

$$\begin{aligned} \|W_2\|_{V(\Omega_{\text{pml}})}^2 & \leq C \sum_{m > kZ/\pi} \int_R^\rho \frac{1}{r} \left[|\hat{w}'_m(r)|^2 - k_m^2 |\hat{w}_m(r)|^2 \right] dr \\ & \leq Cd |\alpha(\rho)|^2 |\beta(\rho)|^2 \sum_{m > kZ/\pi} \int_R^\rho \left[\xi |\hat{w}'_m(r)|^2 - C_0 k_m^2 \eta |\hat{w}_m(r)|^2 \right] dr \\ & \leq Cd |\alpha(\rho)|^2 |\beta(\rho)|^2 \sum_{m > kZ/\pi} \text{Re } \mathcal{A}_m(\hat{w}_m, \hat{w}_m). \end{aligned}$$

Analogously, using (4.24) and the relation $a_{\text{pml}}(W_2, W_2) = \frac{Z}{2} \sum_{m > kZ/\pi} \mathcal{A}_m(\hat{w}_m, \hat{w}_m)$, we deduce that

$$\|W_2\|_{V(\Omega_{\text{pml}})} \leq Cd |\alpha(\rho)|^2 |\beta(\rho)|^2 \|\eta\|_{H^{1/2}(\Gamma_R)}. \quad (4.26)$$

The proof is finished by combining (4.25)–(4.26) and (4.23). \square

Corollary 4.3. *Let \hat{T} be the approximate DtN operator defined in (4.9). There exists a constant $C > 0$ independent of χ_0 and ρ such that*

$$\|\hat{T}\eta\|_{H^{-1/2}(\Gamma_R)} \leq Cd^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 \|\eta\|_{H^{1/2}(\Gamma_R)} \quad \forall \eta \in H_0^{1/2}(\Gamma_R).$$

Proof. Given $\eta \in H_0^{1/2}(\Gamma_R)$, let $w \in H^1(\Omega_{\text{pml}})$ be the solution to (4.10). Define $\mathbf{v} = \left(\frac{1}{r\alpha\beta} \frac{\partial w}{\partial r}, \frac{\alpha}{r\beta} \frac{\partial w}{\partial z} \right)$. From (4.10a) we know that

$$\operatorname{div}_{r,z} \mathbf{v} = \frac{\partial}{\partial r} \left(\frac{1}{r\alpha\beta} \frac{\partial w}{\partial r} \right) + \frac{\partial}{\partial z} \left(\frac{\alpha}{r\beta} \frac{\partial w}{\partial z} \right) = -k^2 \frac{\alpha}{r\beta} w \in L^2(\Omega_{\text{pml}}). \quad (4.27)$$

Let $\mathbf{n} = (1, 0)$ denote the outer normal on Γ_R . Then (4.9) and the trace theorem indicate that

$$\begin{aligned} \|\hat{T}\eta\|_{H^{-1/2}(\Gamma_R)} &= R^2 \left\| \frac{\partial}{\partial r} (r^{-1}w) \right\|_{H^{-1/2}(\Gamma_R)} \\ &\leq R^2 \left\| \frac{1}{r\alpha\beta} \frac{\partial w}{\partial r} \right\|_{H^{-1/2}(\Gamma_R)} + \|w\|_{H^{-1/2}(\Gamma_R)} \\ &= R^2 \|\mathbf{v} \cdot \mathbf{n}\|_{H^{-1/2}(\Gamma_R)} + \|w\|_{H^{-1/2}(\Gamma_R)} \\ &\leq C \left(\|\mathbf{v}\|_{\mathbf{H}(\operatorname{div}, \Omega_{\text{pml}})} + \|w\|_{H^1(\Omega_{\text{pml}})} \right). \end{aligned}$$

Together with (4.27), this yields $\|\hat{T}\eta\|_{H^{-1/2}(\Gamma_R)} \leq C \|w\|_{H^1(\Omega_{\text{pml}})}$. The proof is finished upon using Theorem 4.2. \square

4.3 Estimation of $T - \hat{T}$

Before studying the convergence of the approximate solution \hat{u} of the problem (4.11), the error estimate of $T\eta - \hat{T}\eta$ for any $\eta \in H_0^{1/2}(\Gamma_R)$ will be addressed in this subsection. To do this, we define the wave propagation operator \mathcal{P} which extends η to the exterior of Ω_R in the following way

$$\mathcal{P}(\eta)(r, z) := \frac{r}{R} \sum_{m=1}^{\infty} \frac{H_1^{(1)}(k_m r)}{H_1^{(1)}(k_m R)} \eta_m \sin(m\pi z/Z) \quad \forall r \geq R.$$

In view of (4.4), it is easy to see that $\mathcal{P}(\eta)$ is the solution to the scattering problem

$$\begin{aligned} r \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial}{\partial r} \mathcal{P}(\eta) \right) + \frac{\partial^2}{\partial z^2} \mathcal{P}(\eta) + k^2 \mathcal{P}(\eta) &= 0 \quad \text{in } \Omega \setminus \overline{\Omega_R}, \\ \mathcal{P}(\eta) &= \eta \quad \text{on } \Gamma_R, \\ \lim_{r \rightarrow \infty} \left| \frac{\partial}{\partial r} \mathcal{P}(\eta) - ik \mathcal{P}(\eta) \right| &= 0. \end{aligned}$$

In particular, the exact solution u to the scattering problem (3.6) satisfies $\mathcal{P}(u|_{\Gamma_R}) = u$ in $\Omega \setminus \overline{\Omega_R}$.

Using the complex stretching, we also define a modified wave propagation operator as

$$\tilde{\mathcal{P}}(\eta)(r, z) := \frac{\tilde{r}}{R} \sum_{m=1}^{\infty} \frac{H_1^{(1)}(k_m \tilde{r})}{H_1^{(1)}(k_m R)} \eta_m \sin(m\pi z/Z) \quad \forall r \geq R. \quad (4.28)$$

It is clear that $\tilde{\mathcal{P}}(\eta)(r, z) = \mathcal{P}(\eta)(\tilde{r}, z)$. The chain rule indicates that $\tilde{\mathcal{P}}(\eta)$ satisfies

$$\begin{aligned} \frac{r\beta}{\alpha} \frac{\partial}{\partial r} \left(\frac{1}{r\alpha\beta} \frac{\partial}{\partial r} \tilde{\mathcal{P}}(\eta) \right) + \frac{\partial^2}{\partial z^2} \tilde{\mathcal{P}}(\eta) + k^2 \tilde{\mathcal{P}}(\eta) &= 0 \quad \text{in } \Omega \setminus \overline{\Omega_R}, \\ \tilde{\mathcal{P}}(\eta) &= \eta \quad \text{on } \Gamma_R. \end{aligned}$$

Lemma 4.4. *There exists a constant $C > 0$ independent of ρ and χ_0 such that*

$$\|\tilde{\mathcal{P}}(\eta)\|_{H^{1/2}(\Gamma_\rho)} \leq CR^{-1} |\tilde{\rho}| e^{-0.8\kappa\chi_0 d^2} \|\eta\|_{H^{1/2}(\Gamma_R)}.$$

Proof. We recall [5, Lemma 2.2] for the following estimate

$$\left| H_1^{(1)}(z) \right| \leq e^{-(1-t^2/|z|^2)^{1/2} \operatorname{Im}(z)} \left| H_1^{(1)}(t) \right|, \quad 0 < t \leq |z|, \quad 0 \leq \arg(z) \leq \pi/2.$$

For $1 \leq m < kZ/\pi$, we have $k_m > 0$ and $0 < \arg \tilde{\rho} < \pi/2$. It follows from $R/|\tilde{\rho}| \leq 0.5$ that

$$\left| H_1^{(1)}(k_m \tilde{\rho}) \right| \leq e^{-0.8\kappa\chi_0 d^2} \left| H_1^{(1)}(k_m R) \right|. \quad (4.29)$$

For $m > kZ/\pi$, we have $k_m = \mathbf{i}|k_m|$, $H_1^{(1)}(k_m \tilde{\rho})$ is connected with the modified Bessel function through

$$H_1^{(1)}(k_m \tilde{\rho}) = -\frac{2}{\pi} K_1(|k_m| \tilde{\rho}).$$

Moreover, by [19, eq. (10.32.9)], the modified Bessel function of the m^{th} order satisfies

$$K_1(|k_m| \tilde{\rho}) = \int_0^\infty e^{-|k_m| \tilde{\rho} \cosh t} \cosh(t) dt.$$

We infer that

$$\left| H_1^{(1)}(k_m \tilde{\rho}) \right| \leq \frac{2}{\pi} \int_0^\infty e^{-|k_m| (\operatorname{Re} \tilde{\rho}) \cosh t} \cosh(t) dt \leq e^{-\kappa\chi_0 d^2} \left| H_1^{(1)}(k_m R) \right|. \quad (4.30)$$

Substituting (4.29) and (4.30) into (4.28) shows

$$\|\tilde{\mathcal{P}}(\eta)\|_{H^{1/2}(\Gamma_\rho)}^2 = \frac{|\tilde{\rho}|^2}{R^2} \sum_{m=1}^\infty m \left| \frac{H_1^{(1)}(k_m \tilde{\rho})}{H_1^{(1)}(k_m R)} \right|^2 |\eta_m|^2 \leq \frac{|\tilde{\rho}|^2}{R^2} e^{-1.6\kappa\chi_0 d^2} \|\eta\|_{H^{1/2}(\Gamma_R)}^2.$$

The proof is finished. \square

The error estimates of $T - \hat{T}$ is given in the following corollary.

Corollary 4.5. *For any $\eta \in H^{1/2}(\Gamma_R)$, there exists a constant $C > 0$ independent of ρ and χ_0 such that*

$$\|T\eta - \hat{T}\eta\|_{H^{-1/2}(\Gamma_R)} \leq Cd^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 |\tilde{\rho}| e^{-0.8\kappa\chi_0 d^2} \|\eta\|_{H^{1/2}(\Gamma_R)}. \quad (4.31)$$

Proof. To prove this result, we consider the following problem in the PML region

$$\frac{r\beta}{\alpha} \frac{\partial}{\partial r} \left(\frac{1}{r\alpha\beta} \frac{\partial p}{\partial r} \right) + \frac{\partial^2 p}{\partial z^2} + k^2 p = 0 \quad \text{in } \Omega_{\text{pml}}, \quad (4.32a)$$

$$p = 0 \quad \text{on } \Gamma_R, \quad (4.32b)$$

$$p = 0 \quad \text{on } \{z = 0\} \cup \{z = Z\}, \quad (4.32c)$$

$$p = w \quad \text{on } \Gamma_\rho. \quad (4.32d)$$

It follows analogously from the proof of Theorem 4.2 that there exists a constant $C > 0$ independent of ρ and χ_0 such that

$$\|p\|_{H^1(\Omega_{\text{pml}})} \leq Cd^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 \|w\|_{H^{1/2}(\Gamma_\rho)}.$$

For any $\varphi \in H^1(\Omega_{\text{pml}})$ such that $\varphi = 0$ on Γ_ρ , we obtain

$$a_{\text{pml}}(p, \varphi) + \frac{1}{R} \int_{\Gamma_R} \frac{\partial p}{\partial r} \bar{\varphi} dz = 0.$$

Thus,

$$\left\| \frac{\partial p}{\partial r} \right\|_{H^{-1/2}(\Gamma_R)} \leq C_1 d^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 \|w\|_{H^{1/2}(\Gamma_\rho)}, \quad (4.33)$$

where $C_1 > 0$ is a constant independent of ρ and χ_0 . Now, for any $\eta \in H^{1/2}(\Gamma_R)$, it follows from the definitions of T and \hat{T} that

$$T\eta - \hat{T}\eta = R^2 \frac{\partial}{\partial r} (r^{-1} p) \quad \text{on } \Gamma_R, \quad (4.34)$$

where p is the solution to the Dirichlet problem (4.32) with $w = \tilde{\mathcal{P}}(\eta)$ on Γ_ρ . Then the final estimates (4.31) results by combining (4.33) and (4.34). \square

4.4 Exponential convergence

Now we are ready to show the convergence of the solution \hat{u} to the approximate problem (4.7), or equivalently, problem (4.11). Similar to (3.7), the variational problem of (4.11) is proposed as follows: find $\hat{u} \in V_R$ such that $\hat{u} = u_D$ on Σ_R and

$$\hat{a}(\hat{u}, v) = \int_{\Gamma_{\text{right}}^1} u_N \bar{v} dr \quad \forall v \in V_{R,0}, \quad (4.35)$$

where the sesquilinear form \hat{a} is defined by

$$\hat{a}(u, v) = \int_{\Omega_R} \left[\frac{\partial u}{\partial r} \frac{\partial \bar{v}}{\partial r} + \frac{\partial u}{\partial z} \frac{\partial \bar{v}}{\partial z} - (k^2 + \mathbf{i}\omega\mu\sigma)u\bar{v} \right] \frac{1}{r} dr dz - \frac{1}{R^2} \langle \hat{T}u + u, v \rangle_{\Gamma_R}. \quad (4.36)$$

Theorem 4.6. *Assuming the PML parameters ρ and χ_0 being such that*

$$C_0 := C_{\text{inf}} - C_1 d^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 |\tilde{\rho}| e^{-0.8\kappa\chi_0 d^2} > 0, \quad (4.37)$$

where the constants $C_{\text{inf}} > 0, C_1 > 0$ independent of ρ and χ_0 come from Theorem 3.7 and Corollary 4.5, then there exists a unique solution to the variational problem (4.35). Moreover, there exists a constant $C > 0$ independent of ρ and χ_0 such that

$$\|u - \hat{u}\|_{V_R} \leq C d^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 |\tilde{\rho}| e^{-0.8\kappa\chi_0 d^2} \|\hat{u}\|_{V_R}. \quad (4.38)$$

Proof. It follows from Theorem 3.7 and Corollary 4.5 that there exists constants $C_{\text{inf}} > 0, C_1 > 0$ independent of ρ and χ_0 such that

$$\begin{aligned} \sup_{0 \neq v \in V_{R,0}} \frac{|\hat{a}(u, v)|}{\|v\|_{V_R}} &= \sup_{0 \neq v \in V_{R,0}} \frac{|a(u, v) + R^{-2} \langle (T - \hat{T})u, v \rangle_{\Gamma_R}|}{\|v\|_{V_R}} \\ &\geq \sup_{0 \neq v \in V_{R,0}} \frac{|a(u, v)|}{\|v\|_{V_R}} - R^{-2} \sup_{0 \neq v \in V_{R,0}} \frac{|\langle (T - \hat{T})u, v \rangle_{\Gamma_R}|}{\|v\|_{V_R}} \\ &\geq \left(C_{\text{inf}} - C_1 d^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 |\tilde{\rho}| e^{-0.8\kappa\chi_0 d^2} \right) \|u\|_{V_R}. \end{aligned}$$

Then under the assumption (4.37), the existence and uniqueness of the solution to the variational problem (4.35) follows immediately. It remains to prove the error estimate (4.38). From (3.7) and (4.35), it is easy to see that the error function $e := u - \hat{u} \in V_{R,0}$ satisfies

$$a(e, v) = R^{-2} \langle (T - \hat{T})\hat{u}, v \rangle_{\Gamma_R} \quad \forall v \in V_{R,0}. \quad (4.39)$$

By the inf-sup condition in Theorem 3.7, we have

$$\begin{aligned} \|u - \hat{u}\|_{V_R} &\leq C_{\text{inf}}^{-1} \sup_{0 \neq v \in V_{R,0}} \frac{|a(e, v)|}{\|v\|_{V_R}} \\ &= R^{-2} C_{\text{inf}}^{-1} \sup_{0 \neq v \in V_{R,0}} \frac{|\langle (T - \hat{T})\hat{u}, v \rangle_{\Gamma_R}|}{\|v\|_{V_R}} \\ &\leq C d^6 |\alpha(\rho)|^4 |\beta(\rho)|^2 |\tilde{\rho}| e^{-0.8\kappa\chi_0 d^2} \|\hat{u}\|_{V_R}, \end{aligned}$$

where $C > 0$ is a constant independent of ρ and χ_0 . \square

5 Numerical experiments

In this section, two numerical examples are presented to illustrate the efficiency of our model to simulate the signal propagation in axons. All the parameters are selected in dimensionless type. The finite element method is

utilized for the numerical discretization, for which the error estimates is left for future work, and the particular implementation for the numerical experiments is programmed in Matlab.

In the first example, we test the convergence of the numerical solution arising from the PML truncation and finite element discretization. We consider the following PML problem

$$\begin{aligned} \frac{r\beta}{\alpha} \frac{\partial}{\partial r} \left(\frac{1}{r\alpha\beta} \frac{\partial w}{\partial r} \right) + \frac{\partial^2 w}{\partial z^2} + k^2 w &= 0 \quad \text{in } \Omega', \\ w &= \eta \quad \text{on } \Gamma_{R'}, \\ w &= 0 \quad \text{on } \partial\Omega' \setminus \Gamma_{R'}, \end{aligned}$$

where $\Omega' = [0, \pi] \times [1, 11]$ with the PML region $\Omega_{\text{pml}} = [0, \pi] \times [10, 11]$ and $R = 10$, $R' = 11$. We set $k = 2$, $\chi_0 = 40$ and the exact solution is given by $w = rH_1^{(1)}(k_m r) \sin(mz)$ with $m = 1$. Figure 2 displays the numerical errors in L^2 and H^1 -norms with respect to the finite element meshsize h which clearly shows the second- and first-order convergence, respectively.

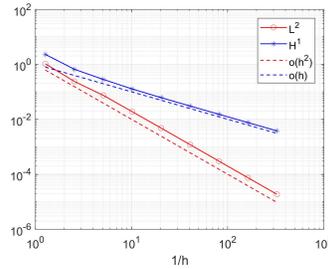


Figure 2: Log-log plot the numerical errors in L^2 and H^1 -norms with respect to the finite element meshsize h .

Next, we test the propagation of an incident signal given on Γ_{left} in the axon and the TE mode is considered. We set

$$u_1(r) = \begin{cases} -J_1(k_c r) & \text{on } \Gamma_{\text{left}} \cap \partial D_1, \\ 0 & \text{otherwise,} \end{cases} \quad u_2(r) = 0, \quad u_N = 0,$$

with $k_c = 2 \times 3.831705970207512$ and choose the parameters

$$(\varepsilon, \sigma) = \begin{cases} (2, 0.2) & \text{in } D_1, \\ (10, 0) & \text{in } D_2, \\ (1.2, 0) & \text{in } D^c, \end{cases} \quad \omega = 5, \quad \mu = 1.$$

The considered axon structures, wherein the axon is wrapped by a long myelin sheath or two separated myelin sheaths or the myelin sheath is absent, are presented in Figure 3. The real parts of the wave fields H_θ and E_z, E_r are plotted in Figures 4-6, respectively. It can be clearly observed that the existence of myelin sheath can gather the electromagnetic fields to propagate mainly in myelin sheath.

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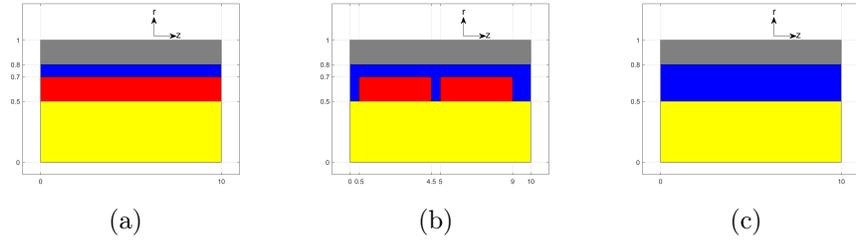


Figure 3: The set-up for simulations wherein the axon is coated by a long myelin sheath (a) or two separated myelin sheaths (b), or the myelin sheath is absent (c). The yellow, red, blue and grey zones represent the regions D_1 , D_2 , D_R^c and Ω_{pml} , respectively.

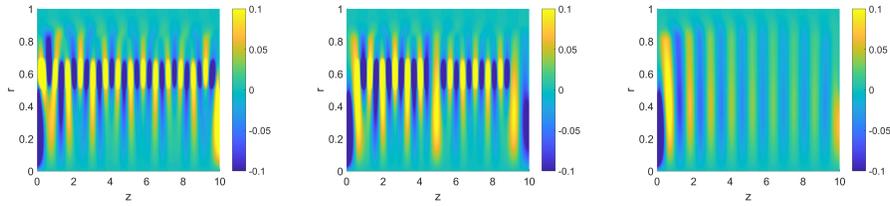


Figure 4: The real part of the magnetic field H_θ for the considered axon structure shown in Figure 3. Left: Figure 3(a), middle: Figure 3(b), right: Figure 3(c).

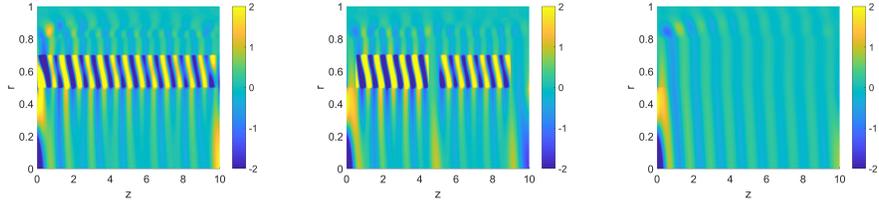


Figure 5: The real part of the magnetic field E_z for the considered axon structure shown in Figure 3. Left: Figure 3(a), middle: Figure 3(b), right: Figure 3(c).

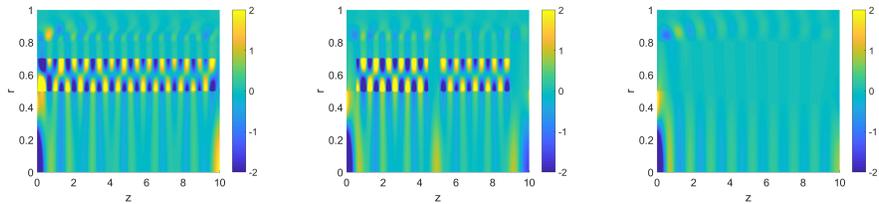


Figure 6: The real part of the magnetic field E_r for the considered axon structure shown in Figure 3. Left: Figure 3(a), middle: Figure 3(b), right: Figure 3(c).

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