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The Method of Fundamental Solutions for Optical Fluorescence

Andreas Karageorghis[1,*] and Daniel Lesnic[2]

[1] *Department of Mathematics and Statistics, University of Cyprus/ Πανεπιστήμιο Κύπρου, P.O.Box 20537, 1678 Nicosia/Λευκωσία, Cyprus/Κύπρος*
[2] *Department of Applied Mathematics, University of Leeds, Leeds LS2 9JT, UK*

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Abstract. In this paper, we develop the method of fundamental solutions (MFS) for solving boundary value problems in the field of optical fluorescence. The governing system of diffusion–absorption equations for the excitation and emission fluences is transformed into a single fourth–order partial differential equation whose fundamental solution can be expressed as the difference of two fundamental solutions of the complex Helmholtz equation. The numerically obtained results confirm the accuracy of the MFS when compared with an available analytical solution. Numerical results are also provided for a physical application in optical fluorescence. Furthermore, extensions to three dimensions along with numerical verification are performed.

AMS subject classifications: 65N80, 65N38

Key words: Optical fluorescence, method of fundamental solutions, elliptic equations.

1 Introduction

Based on the fact that near–infrared light at wavelengths between 700 to 900nm can travel several centimeters into a biological tissue, fluorescence optical tomography has emerged as a suitable molecular imaging tool for anomaly detection, see e.g., [1, 12–14, 18]. In the iterative process of inverse retrieval of a concealed defect in a tissue, a direct solver has to be called repeatedly many times until convergence of a

*Corresponding author.
Emails: andreask@ucy.ac.cy (A. Karageorghis), amt5ld@maths.leeds.ac.uk (D. Lesnic)

nonlinear minimization algorithm is achieved. Prior to this study, the finite element method (FEM) has been utilized and applied adaptively with some success [1, 11, 13, 14]. The FEM has the advantage of dealing with inhomogeneous media, but in many cases the biological properties of tissues as well as the fluorescent properties of contrasting agents employed in molecular imaging are piecewise constant across various layers of material. In these situations it is then possible to apply simpler and faster approximation methods such as the method of fundamental solutions (MFS), which is a versatile meshless boundary collocation technique for solving both direct and inverse boundary value problems [6, 16] without the need of internal domain discretisation. This method, like the boundary element method (BEM) [7, 10], is applicable to problems governed by equations, the partial differential operators of which possess explicitly available fundamental solutions.

The paper is organized as follows. In Section 2 we describe the mathematical model of optical fluorescence and the details of its approximation by the MFS are provided in Section 3. Numerical experiments are presented and analyzed in Section 4 with the three–dimensional extension provided in Section 5. Finally, Section 6 highlights the conclusions of the present study.

2 Mathematical model

The governing equations of photon propagation in a bounded tissue Ω, in the frequency domain, can be obtained as the scattering limit of the full radiative transfer equations [2] and are given by [1, 11]

$$-\nabla\cdot(D_{\rm x}\nabla u)+\kappa_{\rm x}u=0 \qquad \text{in} \;\; \Omega, \tag{2.1a}$$

$$-\nabla\cdot(D_{\rm m}\nabla v)+\kappa_{\rm m}v=\beta_{\rm x}u \qquad \text{in} \;\; \Omega, \tag{2.1b}$$

where u is the excitation (incident) light fluence, v is the emission (fluorescence) light fluence, $\kappa_{\rm x}$ and $\kappa_{\rm m}$ are the total photon absorption coefficients at excitation (subscript x) and emission (subscript m) wavelengths, respectively, $D_{\rm x}$ and $D_{\rm m}$ are the photon diffusion coefficients at excitation and emission wavelengths, respectively, and $\beta_{\rm x}$ is a coupling coefficient defined below in Eq. (2.3). The boundary conditions associated to (2.1a) and (2.1b) are of Robin type and given by

$$2D_{\rm x}\frac{\partial u}{\partial n}+\gamma u+S=0 \qquad \text{on} \;\; \partial\Omega, \tag{2.2a}$$

$$2D_{\rm m}\frac{\partial v}{\partial n}+\gamma v=0 \qquad \text{on} \;\; \partial\Omega, \tag{2.2b}$$

where $\boldsymbol{n}$ is the outward unit normal to $\partial\Omega$, γ is a constant depending on the optical refractive index mismatch at the boundary [8] and S is an excitation source.