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Numerical Simulation of Flow in Liquid Crystals using MATLAB software

M. Fallahpour, S. McKee, and E.B. Weinmüller

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Numerical Simulation of Flow in Liquid Crystals using MATLAB Software

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Abstract

Contents

1 Introduction **2**

2 Notation **2**

3 Linear problem **3**
3.1 Transforming the system 3
3.2 Solving the linear system BVP (4)–(7) 3
3.2.1 First solution approach 3
3.2.2 Second solution approach 8
3.2.3 Solutions to the linear problem (4)–(7) 10
3.3 Calculation with `bvpsuite2.0` 11

4 Nonlinear problem (1)–(4) **16**

5 Conclusions **16**

1 Introduction

We consider the following system of differential equations for the unknown functions $\theta(z)$, $\delta(z)$, and $u(z)$ [3]:

$$
\begin{aligned}
&M(\theta,\delta)\sin(\theta-\delta) - K_1^a\cos(\theta)\frac{\mathrm{d}^2}{\mathrm{d}z^2}\sin(\theta) \\
&\quad + \frac{\mathrm{d}u}{\mathrm{d}z}\left[a_3\cos(\theta)^2 - \ -a_2\sin(\theta)^2 + \kappa_1\cos(\theta-\delta)\right] = 0, && (1)\\
&a - J_{3,3} - \tilde{t}_{13,3} = 0, && (2)\\
&u + \lambda_p J_{3,3} = 0, && (3)
\end{aligned}
$$

where

$$
\begin{aligned}
&M(\theta,\delta) = B_1\cos(\theta-\delta) - B_0\left[\sec(\delta) + cos(\theta-\delta) - 2\right],\\
&J_3 = \cos(\delta)^2\left[K_1^a\cos(\delta)\frac{\mathrm{d}^2}{\mathrm{d}z^2}\sin(\delta) + M(\theta,\delta)\sin(\theta-\delta)\right] - \\
&\quad - B_0\sin(\delta)\left[\sec(\delta) + \cos(\theta-\delta) - 2\right],\\
&\tilde{t}_{13} = \frac{1}{2}u'(a_4 + a_5 - a_2 + \tau_2) + \frac{1}{4}u'\left[a_1\sin(2\theta)^2 + \tau_1\sin(2\delta)^2\right] + u'\left[\kappa_1\cos(\theta+\delta) + \right.\\
&\quad \left. + \kappa_6\cos(\theta-\delta) + (a_2+a_3)\cos(\theta)^2\right] + \frac{1}{2}u'\left[\kappa_2\ sin(\theta+\delta)^2 + \right.\\
&\quad \left. + \kappa_3\sin(2\theta)\sin(2\delta)\right] + u'\sin(\theta+\delta)\left[\kappa_4\sin(2\theta) + \kappa_5\sin(2\delta)\right].
\end{aligned}
$$

Here, K_1^a, λ_p, a_1 to a_5, B_0, B_1, τ_1, τ_2, and κ_1 to κ_6 are constant parameters. Moreover, we use following notation:

$$
J_{3,3} = \frac{\mathrm{d}}{\mathrm{d}z}J_3, \quad \tilde{t}_{13,3} = \frac{\mathrm{d}}{\mathrm{d}z}\tilde{t}_{13}.
$$

Equations (1)–(3) are subject to following boundary conditions:

$$
u(\pm d/2) = 0, \quad \theta(\pm d/2) = \pm\theta_0, \quad \delta(\pm d/2) = \pm\delta_0, \quad \delta''(0) = 0. \tag{4}
$$

We first find the solution to the linearized system of equations derived from (1)–(3) under the assumption that u, θ and δ and their derivatives are small. With the solution to this linear system of equations, we will have found a good starting guess for the numerical solution of the nonlinear system (1)–(3). Respective numerical simulation will be carried out using the MATLAB code `bvpsuite2.0` [4, 1].

2 Notation

As always we write

$$
\cosh(x) = \frac{e^x + e^{-x}}{2}, \quad \sinh(x) = \frac{e^x - e^{-x}}{2}
$$

and

$$
\operatorname{sech}(x) = \cosh(x)^{-1}, \quad \operatorname{csch}(x) = \sinh(x)^{-1}.
$$

3 Linear problem

3.1 Transforming the system

We transform equations (1)–(3) into a linear system of equations under the assumption that u, θ and δ and their derivatives are small. We use the approximations $\sin(x) \approx x$ and $\cos(x) \approx 1$ for small x. Then the following three equations follow:

$$B_1(\theta - \delta) - K_1^a \theta'' + u'(a_3 + \kappa_1) = 0, \tag{5}$$
$$K_1^a \delta''' + B_1(\theta' - \delta') + \eta u'' - a = 0, \tag{6}$$
$$u + \lambda_p \left[K_1^a \delta''' + B_1(\theta' - \delta')\right] = 0, \tag{7}$$

where $2\eta = a_2 + a_4 + a_5 + \tau_2 + 2(a_3 + \kappa_1 + \kappa_6)$.

These differential equations are subject to the boundary conditions (4). Now, we provide the exact solution of the BVP (4)–(7).

3.2 Solving the linear system BVP (4)–(7)

We first multiply (7) by λ_p^{-1} and substract from (6). This yields

$$\begin{aligned}
&B_1(\theta - \delta) - K_1^a \theta'' + u'(a_3 + \kappa_1) = 0,\\
&u + \lambda_p \left[K_1^a \delta''' + B_1(\theta' - \delta')\right] = 0,\\
&\eta u'' - u\lambda_p^{-1} - a = 0,
\end{aligned}$$

or equivalently,

$$K_1^a \theta'' = B_1(\theta - \delta) + u'(a_3 + \kappa_1), \tag{8}$$
$$\lambda_p K_1^a \delta''' = -u - \lambda_p B_1(\theta' - \delta'), \tag{9}$$
$$\eta u'' = u\lambda_p^{-1} + a. \tag{10}$$

3.2.1 First solution approach

Here, we reconstruct the reasoning from [3]. Let us define x and b as follows:

$$x := (\theta, \theta', \delta, \delta', \delta'', u, u')^T, \quad b := (0, 0, 0, 0, 0, 0, a/\eta)^T,$$

and transform system (8)–(10) into its first order form,

$$\frac{\mathrm{d}x}{\mathrm{d}z} = Ax + b, \tag{11}$$

where A is the 7×7 matrix

$$A := \begin{pmatrix}
0 & 1 & 0 & 0 & 0 & 0 & 0\\
B_1/K_1^a & 0 & -B_1/K_1^a & 0 & 0 & 0 & (a_3 + \kappa_1)/K_1^a\\
0 & 0 & 0 & 1 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 1 & 0 & 0\\
0 & -B_1/K_1^a & 0 & B_1/K_1^a & 0 & -1/K_1^a\lambda_p & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 1\\
0 & 0 & 0 & 0 & 0 & 1/\eta\lambda_p & 0
\end{pmatrix}.$$

The characteristic polynomial of A is

$$\chi_A(t) := \det(A - tE_7) = t^3 \left(t^2 - \frac{1}{\eta\lambda_p}\right)\left(t^2 - \frac{2B_1}{K_1^a}\right).$$

Thus, $\pm\lambda_1$, $\pm\lambda_2$ and $\lambda_3 = 0$ are eigenvalues of A, where

$$\lambda_1 := \frac{1}{\sqrt{\eta\lambda_p}}, \quad \lambda_2 := \sqrt{\frac{2B_1}{K_1^a}}.$$

The algebraic multiplicity of $\lambda_3 = 0$ is three, but its geometrical multiplicity is one. Therefore, we need to find three generalized eigenvectors of A associated with $\lambda_3 = 0$ that span the respective generalized eigenspaces. We solve the three equations

$$Ah_1 = 0, \quad Ah_2 = h_1, \quad Ah_3 = h_2,$$

we obtain

$$h_1 = (1,0,1,0,0,0,0)^T, \quad h_2 = (0,1,0,1,0,0,0)^T, \quad h_3 = \left(2\lambda_2^{-2},0,0,0,1,0,0\right)^T.$$

We now have three solutions of (11),

$$x_1 = h_1, \quad x_2 = h_1 + h_2 + zh_1, \quad x_3 = h_1 + h_2 + h_3 + z(h_1 + h_2) + \frac{z^2}{2}h_1.$$

The vectors h_1, h_2, h_3 and the eigenvectors $v_1^{\pm}$, $v_2^{\pm}$, associated with the eigenvalues $\pm\lambda_1$ and $\pm\lambda_2$, are seven linearly independent vectors which span $\mathbb{R}^7$. We use them to derive the fundamental solution matrix $R(z)$.

Variation of constants now yields the general solution of (11),

$$x(z) = R(z)c + R(z)\int_{z_0}^{z} R^{-1}(s)\, b\, \mathrm{d}s, \tag{12}$$

where $c \in \mathbb{R}^7$. We now define $R(z)$,

$$R(z) := Q(z)\mathrm{diag}(e^{\lambda_1 z}, e^{-\lambda_1 z}, 1, e^{\lambda_2 z}, e^{-\lambda_2 z}, 1, 1),$$

where $Q(z)$ is a matrix containing all eigenvectors and generalized eigenvectors of A,

$$Q(z) = \begin{pmatrix} \beta_1 & \beta_1 & 1 & -1 & -1 & \frac{1}{2}z^2 + z + 1 + 2\lambda_2^{-2} & z+1 \\ \lambda_1\beta_1 & -\lambda_1\beta_1 & 0 & -\lambda_2 & \lambda_2 & z+1 & 1 \\ 1 & 1 & 1 & 1 & 1 & \frac{1}{2}z^2 + z + 1 & z+1 \\ \lambda_1 & -\lambda_1 & 0 & \lambda_2 & -\lambda_2 & z+1 & 1 \\ \lambda_1^2 & \lambda_1^2 & 0 & \lambda_2^2 & \lambda_2^2 & 1 & 0 \\ -\lambda_1^2\beta_2 & \lambda_1^2\beta_2 & 0 & 0 & 0 & 0 & 0 \\ -\lambda_1^3\beta_2 & -\lambda_1^3\beta_2 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

with

$$\beta_1 = \frac{B_1\eta\lambda_p(a_3 + \kappa_1 - \eta) - K_1^a(a_3 + \kappa_1)}{\eta[K_1^a + B_1\lambda_p(a_3 + \kappa_1 - \eta)]}, \quad \beta_2 = \frac{(K_1^a)^2(\lambda_1^2 - \lambda_2^2)}{\eta\lambda_1^3[K_1^a + B_1\lambda_p(a_3 + \kappa_1 - \eta)]}.$$

First we note that due to the form of b, we only need the 7th column of R^{-1}. We compute this column and obtain

$$R^{-1}(z)\,b = \frac{a}{\eta}\begin{pmatrix} \left(-\frac{1}{2\lambda_1^3\beta_2}\right)e^{-\lambda_1 z} \\ \left(-\frac{1}{2\lambda_1^3\beta_2}\right)e^{\lambda_1 z} \\ \frac{1+\beta_1}{2\lambda_1^3\beta_2} + \sigma\left(\frac{1}{2}z^2 + z - \lambda_2^{-2}\right) \\ \tau e^{-\lambda_2 z} \\ \tau e^{\lambda_2 z} \\ \sigma \\ -(z+1)\sigma \end{pmatrix},$$

where

$$\sigma := \frac{2\lambda_1^2 - \lambda_2^2 + \lambda_2^2\beta_1}{4\lambda_1^3\beta_2}, \quad \tau := \frac{2\lambda_1^2 + \lambda_2^2 - \lambda_2^2\beta_1}{8\lambda_1^3\lambda_2^2\beta_2}.$$

Next, we integrate from z_0 to z,

$$\int_{z_0}^{z} R^{-1}\,b\,\mathrm{d}s = \frac{a}{\eta}\begin{pmatrix} \frac{1}{2\lambda_1^4\beta_2}\left(e^{-\lambda_1 z} - e^{-\lambda_1 z_0}\right) \\ -\frac{1}{2\lambda_1^4\beta_2}\left(e^{\lambda_1 z} - e^{\lambda_1 z_0}\right) \\ \frac{1+\beta_1}{2\lambda_1^3\beta_2}\Delta_1^z + \sigma\left(\frac{1}{6}\Delta_3^z + \frac{1}{2}\Delta_2^z - \lambda_2^{-2}\Delta_1^z\right) \\ -\frac{\tau}{\lambda_2}\left(e^{-\lambda_2 z} - e^{-\lambda_2 z_0}\right) \\ \frac{\tau}{\lambda_2}\left(e^{\lambda_2 z} - e^{\lambda_2 z_0}\right) \\ \sigma\Delta_1^z \\ -\left(\frac{1}{2}\Delta_2^z + \Delta_1^z\right)\sigma \end{pmatrix},$$

where $\Delta_n^z := z^n - z_0^n$ with $n \in \mathbb{N}$. Setting $z_0 = 0$ and $z = \pm d/2$ yields

$$\int_0^{\pm\frac{d}{2}} R^{-1}(s)b\mathrm{d}s = \frac{a}{\eta}\begin{pmatrix} \frac{e^{\mp\lambda_1 d/2}-1}{2\lambda_1^4\beta_2} \\ -\frac{e^{\pm\lambda_1 d/2}-1}{2\lambda_1^4\beta_2} \\ \pm\frac{1+\beta_1}{4\lambda_1^3\beta_2}d + \sigma\left(\pm\frac{1}{48}d^3 + \frac{1}{8}d^2 \mp \frac{d}{2\lambda_2^2}\right) \\ -\frac{\tau}{\lambda_2}\left(e^{\mp\lambda_2 d/2} - 1\right) \\ \frac{\tau}{\lambda_2}\left(e^{\pm\lambda_2 d/2} - 1\right) \\ \pm\frac{\sigma}{2}d \\ -\left(\frac{1}{8}d^2 \pm \frac{d}{2}\right)\sigma \end{pmatrix}.$$

With conditions (4) we have,

$$x(0) = (\theta(0), \theta'(0), \delta(0), \delta'(0), 0, u(0), u'(0))^T,$$
$$x(\pm d/2) = (\pm\theta_0, \theta'(\pm d/2), \pm\delta_0, \delta'(\pm d/2), \delta''(\pm d/2), 0, u'(\pm d/2))^T,$$

and due to (12), we can write

$$\delta''(0) = 0 = \lambda_1^2 c_1 + \lambda_1^2 c_2 + \lambda_2^2 c_4 + \lambda_2^2 c_5 + c_6, \tag{13}$$

$$u(\pm d/2) = 0 = \lambda_1^2 \beta_2 \left(-e^{\pm\lambda_1 d/2} c_1 + e^{\mp\lambda_1 d/2} c_2\right) + \frac{a\cosh(\lambda_1 d/2) - a}{\eta \lambda_1^2}, \tag{14}$$

$$\begin{aligned}\delta(\pm d/2) = \pm\delta_0 = {} & e^{\pm\lambda_1 d/2} c_1 + e^{\mp\lambda_1 d/2} c_2 + c_3 + e^{\pm\lambda_2 d/2} c_4 + e^{\mp\lambda_1 d/2} c_5 + \\ & + \left(\frac{1}{8} d^2 \pm \frac{d}{2} + 1\right) c_6 + \left(\pm\frac{d}{2} + 1\right) c_7 + \frac{a}{\eta}\left[\mp \frac{1}{\lambda_1^4 \beta_2} \sinh(\lambda_1 d/2) \pm \right. \\ & \left. \pm \frac{2\tau}{\lambda_2} \sinh(\lambda_2 d/2) \pm \frac{1+\beta_1}{4\lambda_1^3 \beta_2} d + \sigma\left(\pm\frac{1}{48} d^3 \mp \frac{1}{2\lambda_2^2} d\right)\right],\end{aligned} \tag{15}$$

$$\begin{aligned}\theta(\pm d/2) = \pm\theta_0 = {} & \beta_1 e^{\pm\lambda_1 d/2} c_1 + \beta_1 e^{\mp\lambda_1 d/2} c_2 + c_3 - e^{\pm\lambda_2 d/2} c_4 - e^{\mp\lambda_1 d/2} c_5 + \\ & + \left(\frac{1}{8} d^2 \pm \frac{d}{2} + 1 + \frac{2}{\lambda_2^2}\right) c_6 + \left(\pm\frac{d}{2} + 1\right) c_7 + \frac{a}{\eta}\left[\mp \frac{\beta_1}{\lambda_1^4 \beta_2} \sinh(\lambda_1 d/2) \mp \right. \\ & \left. \mp \frac{2\tau}{\lambda_2} \sinh(\lambda_2 d/2) \pm \frac{1+\beta_1}{4\lambda_1^3 \beta_2} d + \sigma\left(\pm\frac{1}{48} d^3 \pm \frac{1}{2\lambda_2^2} d\right)\right].\end{aligned} \tag{16}$$

It follows from (14) that

$$u(d/2) - u(-d/2) = \lambda_1^2 \beta_2 \left(\left(e^{-\lambda_1 d/2} - e^{\lambda_1 d/2}\right) c_1 + \left(e^{-\lambda_1 d/2} - e^{\lambda_1 d/2}\right) c_2\right) = 0,$$

and thus, $c_2 = -c_1$. Finally, using (14), we find c_1 and c_2,

$$c_1 = -c_2 = -\frac{a\,\mathrm{sech}(\lambda_1 d/2) - a}{2\lambda_1^4 \eta \beta_2}.$$

We now insert c_1 into (13), (15), and (16) and obtain

$$\delta''(0) = 0 = \lambda_2^2 c_4 + \lambda_2^2 c_5 + c_6, \tag{17}$$

$$\begin{aligned}\delta(\pm d/2) = \pm\delta_0 = {} & c_3 + e^{\pm\lambda_2 d/2} c_4 + e^{\mp\lambda_1 d/2} c_5 + \left(\frac{1}{8} d^2 \pm \frac{d}{2} + 1\right) c_6 + \left(\pm\frac{d}{2} + 1\right) c_7 + \\ & + \frac{a}{\eta}\left[\mp \frac{1}{\lambda_1^4 \beta_2} \sinh(\lambda_1 d/2) \pm \frac{2\tau}{\lambda_2} \sinh(\lambda_2 d/2) \pm \frac{1+\beta_1}{4\lambda_1^3 \beta_2} d + \right. \\ & \left. + \sigma\left(\pm\frac{1}{48} d^3 \mp \frac{1}{2\lambda_2^2} d\right) \mp \frac{\tanh(\lambda_1 d/2) - \sinh(\lambda_1 d/2)}{\lambda_1^4 \beta_2}\right],\end{aligned} \tag{18}$$

$$\begin{aligned}\theta(\pm d/2) = \pm\theta_0 = {} & c_3 - e^{\pm\lambda_2 d/2} c_4 - e^{\mp\lambda_1 d/2} c_5 + \left(\frac{1}{8} d^2 \pm \frac{d}{2} + 1 + \frac{2}{\lambda_2^2}\right) c_6 + \\ & + \left(\pm\frac{d}{2} + 1\right) c_7 + \frac{a}{\eta}\left[\mp \frac{\beta_1}{\lambda_1^4 \beta_2} \sinh(\lambda_1 d/2) \mp \frac{2\tau}{\lambda_2} \sinh(\lambda_2 d/2) \pm \right. \\ & \left. \pm \frac{1+\beta_1}{4\lambda_1^3 \beta_2} d + \sigma\left(\pm\frac{1}{48} d^3 \pm \frac{1}{2\lambda_2^2} d\right) \mp \beta_1 \frac{\tanh(\lambda_1 d/2) - \sinh(\lambda_1 d/2)}{\lambda_1^4 \beta_2}\right].\end{aligned} \tag{19}$$

Subtracting (19) from (18) results in

$$\begin{aligned}\pm\delta_0 \mp \theta_0 = {} & 2e^{\pm\lambda_2 d/2} c_4 + 2e^{\mp\lambda_2 d/2} c_5 - \frac{2}{\lambda_p^2} c_6 + \frac{a}{\eta}\left[\frac{\mp 1 \pm \beta_1}{\lambda_1^4 \beta_2} \sinh(\lambda_1 d/2) \pm \right. \\ & \left. \pm \frac{4\tau}{\lambda_2} \sinh(\lambda_2 d/2) + \sigma\left(\mp\frac{1}{\lambda_2^2} d\right) + (\mp 1 \pm \beta_1) \frac{\tanh(\lambda_1 d/2) - \sinh(\lambda_1 d/2)}{\lambda_1^4 \beta_2}\right].\end{aligned} \tag{20}$$

Next, we multiply (17) by $2/\lambda_2^2$ and add to each of the equations in (20). Then, we add the resulting equations to each other and have,

$$\delta_0 - \theta_0 + (-\delta_0 + \theta_0) = 0 = 2\left(e^{\lambda_2 d/2} + e^{-\lambda_2 d/2} + 2\right) c_4 + 2\left(e^{-\lambda_2 d/2} + e^{\lambda_2 d/2} + 2\right) c_5,$$

wherefrom $c_5 = -c_4$ follows. Moreover, $c_6 = 0$ by (17). Using (20), we find the following expressions for c_4 and c_5:

$$c_4 = -c_5 = \frac{\delta_0 - \theta_0}{4} \operatorname{csch}(\lambda_2 d/2) + \frac{a}{\eta}\left[\frac{1-\beta_1}{4\lambda_1^4\beta_2}\sinh(\lambda_1 d/2)\operatorname{csch}(\lambda_2 d/2) - \frac{\tau}{\lambda_2} + \right.$$
$$\left. + \sigma\frac{\operatorname{csch}(\lambda_2 d/2)}{4\lambda_2^2} d + \operatorname{csch}(\lambda_2 d/2)(1-\beta_1)\frac{\tanh(\lambda_1 d/2) - \sinh(\lambda_1 d/2)}{4\lambda_1^4\beta_2}\right],$$

Adding (18) and (19) gives

$$\pm\,\delta_0 \pm \theta_0 = 2c_3 + (\pm d + 2)\, c_7 + \frac{a}{\eta}\left[\mp\frac{1+\beta_1}{\lambda_1^4\beta_2}\sinh(\lambda_1 d/2) \pm \frac{1+\beta_1}{2\lambda_1^3\beta_2} d + \right.$$
$$\left. + \sigma\left(\pm\frac{1}{24}d^3\right) \mp (1+\beta_1)\frac{\tanh(\lambda_1 d/2) - \sinh(\lambda_1 d/2)}{\lambda_1^4\beta_2}\right]. \tag{21}$$

We now consider

$$\delta_0 + \theta_0 - (-\delta_0 - \theta_0) = 2dc_7 + \frac{a}{\eta}\left[-\frac{2(1+\beta_1)}{\lambda_1^4\beta_2}\sinh(\lambda_1 d/2) + \frac{1+\beta_1}{\lambda_1^3\beta_2} d + \right.$$
$$\left. + \sigma\left(\frac{1}{12}d^3\right) - 2(1+\beta_1)\frac{\tanh(\lambda_1 d/2) - \sinh(\lambda_1 d/2)}{\lambda_1^4\beta_2}\right].$$

wherefrom, we obtain c_7,

$$c_7 = \frac{1}{d}(\delta_0 + \theta_0) + \frac{a}{d\eta}\left[\frac{(1+\beta_1)}{\lambda_1^2\beta_2}\sinh(\lambda_1 d/2) - \frac{1+\beta_1}{2\lambda_1^3\beta_2} d - \sigma\left(\frac{1}{24}d^3\right) + \right.$$
$$\left. + (1+\beta_1)\frac{\tanh(\lambda_1 d/2) - \sinh(\lambda_1 d/2)}{\lambda_1^4\beta_2}\right].$$

We insert c_7 into (21) and after some easy calculations $c_3 = -c_7$ follows.

This means that we now know all entries of the vector c and the solution $\theta(z)$, $\delta(z)$ and $u(z)$ of the system (5)–(7) subject to boundary conditions (4) follows,

$$\theta(z) = 2\beta_1\sinh(\lambda_1 z)c_1 - 2\sinh(\lambda_2 z)c_4 + zc_7 + \frac{a}{\eta}\left[-\beta_1\frac{\sinh(\lambda_1 z)}{\lambda_1^4\beta_2} - \frac{2\tau}{\lambda_2}\sinh(\lambda_2 z) + \right.$$
$$\left. + \frac{1+\beta_1}{2\lambda_1^3\beta_2} z + \sigma\left(\frac{1}{6}z^3 + z\lambda_2^{-2}\right)\right],$$
$$\delta(z) = 2\sinh(\lambda_1 z)c_1 + 2\sinh(\lambda_2 z)c_4 + zc_7 + \frac{a}{\eta}\left[-\frac{\sinh(\lambda_1 z)}{\lambda_1^4\beta_2} + \frac{2\tau}{\lambda_2}\sinh(\lambda_2 z) + \right.$$
$$\left. + \frac{1+\beta_1}{2\lambda_1^3\beta_2} z + \sigma\left(\frac{1}{6}z^3 - z\lambda_2^{-2}\right)\right],$$
$$u(z) = a\lambda_p\left[\frac{\cosh(\lambda_1 z)}{\cosh(\lambda_1 d/2)} - 1\right].$$

We have verified by hand and using Maple that the above functions satisfy equations (5)–(7) and boundary conditions (4).

3.2.2 Second solution approach

The only unknown in (10) is u, so we solve this equation for u and obtain

$$u(z) = q_1 e^{\lambda_1 z} + q_2 e^{-\lambda_1 z} - a\lambda_p,$$

where $\lambda_1 = \frac{1}{\sqrt{\eta\lambda_p}}$, as in the first approach, and q_1 and q_2 are constant. From the boundary conditions $u(\pm d/2) = 0$ we know that

$$q_1 e^{\pm\lambda_1 d/2} + q_2 e^{\mp\lambda_1 d/s} = 0 \quad \Rightarrow \quad 2(q_1 - q_2)\underbrace{\sinh(\lambda_1 d/2)}_{\neq 0 \text{ since } d\neq 0} = 0 \quad \Rightarrow \quad q_1 = q_2.$$

With this result and $u(\pm d/2) = 0$ we can now write u in the following way:

$$u(z) = q\cosh(\lambda_1 z) - a\lambda_p, \tag{22}$$

where $q := 2q_1 = 2q_2 = a\lambda_p \operatorname{sech}(\lambda_1 d/2)$.

Now we differentiate (5) and subtract the result from (6),

$$\delta''' + \theta''' = \frac{1}{K_1^a}\left[a - u''(\eta - a_3 - \kappa_1)\right] = \frac{1}{K_1^a}\left[a - q\lambda_1^2\nu\cosh(\lambda_1 z)\right],$$

where $\nu := \eta - a_3 - \kappa_1$. We integrate this ODE three times and obtain

$$\delta + \theta = \frac{1}{K_1^a}\left[\frac{a}{6}z^3 - \frac{q\nu}{\lambda_1}\sinh(\lambda_1 z)\right] + q_3 z^2 + q_4 z + q_5, \tag{23}$$

where q_3, q_4 and q_5 are constant.

Replacing $\theta - \delta$ by $-\theta - \delta + 2\theta$ in (5) and with the previous result an ODE for θ follows,

$$\begin{aligned}
&B_1(-\theta - \delta + 2\theta) - K_1^a\theta'' + u'(a_3 + \kappa_1) = 0\\
&\Rightarrow \quad K_1^a\theta'' - 2B_1\theta = -B_1\left(\frac{1}{K_1^a}\left[\frac{a}{6}z^3 - \frac{q\nu}{\lambda_1}\sinh(\lambda_1 z)\right] + q_3 z^2 + q_4 z + q_5\right) +\\
&\qquad\qquad + q\lambda_1\sinh(\lambda_1 z)(a_3 + \kappa_1),\\
&\Rightarrow \quad \theta'' = \lambda_2^2\theta - \frac{\lambda_2^2}{2}\left(\frac{a}{6K_1^a}z^3 + q_3 z^2 + q_4 z + q_5\right) + \frac{q\left(\lambda_2^2\nu + 2\lambda_1^2(a_3 + \kappa_1)\right)}{2K_1^a\lambda_1}\sinh(\lambda_1 z),
\end{aligned}$$

where $\lambda_2 = \sqrt{\frac{2B_1}{K_1^a}}$.

Let $\omega \in C^2[-d/2, d/2]$ and let $r \neq 0$, $s \neq 0$, and t be constants. Consider

$$\omega'' = s\omega + r\sinh(tz).$$

Then,

$$\omega(z) = k_1 e^{\sqrt{s}z} + k_2 e^{-\sqrt{s}z} + \begin{cases} \frac{r}{2t}\cosh(z)z, & \text{if } s = t^2 \text{ and } r \neq 0,\\ 0, & \text{if } t = 0 \text{ or } r = 0 \text{ and } s \text{ arbitrary},\\ \frac{rs}{t^2 - s}\sinh(tz), & \text{else,}\end{cases}$$

with arbitrary constants k_1 and k_2.

From the chart in [3, p.1829], we see that $\lambda_1 \approx 2$ and $\lambda_2 \approx 10^9$, and therefore, we assume that $\lambda_1^2 < \lambda_2^2$.

We now can specify $\theta(z)$,

$$\theta(z) = \frac{a}{12K_1^a}z^3 + \frac{q_3}{2}z^2 + \frac{2q_4B_1 + a}{4B_1}z + \frac{B_1q_5 + K_1^a q_3}{2B_1} + q_6e^{\lambda_2 z} + q_7e^{-\lambda_2 z} + \\ + \frac{q\left(\lambda_2^2\nu + 2\lambda_1^2(a_3 + \kappa_1)\right)}{2K_1^a\lambda_1\left(\lambda_1^2 - \lambda_2^2\right)}\sinh(\lambda_1 z), \tag{24}$$

where q_6 and q_7 are constants. With (24) and (23), we find $\delta(z)$,

$$\delta(z) = \frac{a}{12K_1^a}z^3 + \frac{q_3}{2}z^2 + \frac{2q_4B_1 - a}{4B_1}z + \frac{B_1q_5 - K_1^a q_3}{2B_1} - q_6e^{\lambda_2 z} - q_7e^{-\lambda_2 z} + \\ + \frac{q\left(\lambda_2^2\nu - 2\lambda_1^2(\nu + a_3 + \kappa_1)\right)}{2K_1^a\lambda_1\left(\lambda_1^2 - \lambda_2^2\right)}\sinh(\lambda_1 z). \tag{25}$$

Finally, we have to choose the constants in such a way that u, δ, and θ, given in (22), (24), and (25), respectively, satisfy the boundary conditions in (4).

From (23) and $\delta''(0) = 0$, we conclude that $\theta''(0) = 2q_3$. Therefore, when we differentiate (24) twice,

$$2q_3 = q_3 + \lambda_2^2 q_6 + \lambda_2^2 q_7 \quad \Rightarrow \quad q_3 = \lambda_2^2 q_6 + \lambda_2^2 q_7 \tag{26}$$

follows. Moreover, (23) and conditions $\delta(\pm d/2) + \theta(\pm d/2) = \pm\delta_0 \pm \theta_0$, imply

$$2\delta_0 + 2\theta_0 = \frac{1}{K_1^a}\left[\frac{a}{24}d^3 - \frac{2q\nu}{\lambda_1}\sinh(\lambda_1 d/2)\right] + q_4 d \;\Rightarrow \\ q_4 = \frac{2}{d}(\delta_0 + \theta_0) - \frac{1}{dK_1^a}\left[\frac{a}{24}d^3 - \frac{2q\nu}{\lambda_1}\sinh(\lambda_1 d/2)\right]$$

and

$$\delta_0 + \theta_0 - \delta_0 - \theta_0 = 0 = \frac{q_3}{2}d^2 + q_5 \quad \Rightarrow \quad q_5 = -\frac{q_3}{2}d^2.$$

By (24), (25), (26) and the boundary conditons $\theta(\pm d/2) = \pm\theta_0$, $\delta(\pm d/2) = \pm\delta_0$,

$$\theta_0 - \delta_0 = 2q_6\left(1 + e^{\lambda_2^2\frac{d}{2}}\right) + 2q_7\left(1 + e^{-\lambda_2^2\frac{d}{2}}\right) + \frac{ad}{4B_1} + \frac{q\lambda_1^2\left(2a_3 + 2\kappa_1 + \nu\right)}{K_1^a\lambda_1\left(\lambda_1^2 - \lambda_2^2\right)}\sinh\left(\lambda_1\frac{d}{2}\right), \\ -\theta_0 + \delta_0 = 2q_6\left(1 + e^{-\lambda_2^2\frac{d}{2}}\right) + 2q_7\left(1 + e^{\lambda_2^2\frac{d}{2}}\right) - \frac{ad}{4B_1} + \frac{q\lambda_1^2\left(2a_3 + 2\kappa_1 + \nu\right)}{K_1^a\lambda_1\left(\lambda_1^2 - \lambda_2^2\right)}\sinh\left(-\lambda_1\frac{d}{2}\right),$$

and addition of those two lines yields,

$$0 = 4\left[1 + \cosh\left(\lambda_2^2\frac{d}{2}\right)\right](q_6 + q_7) \quad \Rightarrow \quad q_6 = -q_7.$$

Thus $q_3 = q_5 = 0$. The value of q_6 can be deduced from the above lines.

To summarize, we have

$$\begin{aligned}
q &= 2q_1 = 2q_2 = a\lambda_p \operatorname{sech}(\lambda_1 d/2),\\
q_3 &= q_5 = 0,\\
q_4 &= \frac{2}{d}(\delta_0 + \theta_0) - \frac{1}{dK_1^a}\left[\frac{a}{24}d^3 - \frac{2q\nu}{\lambda_1}\sinh(\lambda_1 d/2)\right],\\
q_6 &= -q_7 = -\operatorname{csch}(\lambda_2 d/2)\left[\frac{\delta_0 - \theta_0}{4} + \frac{ad}{16B_1} + \frac{q\lambda_1^2(2\eta - \nu)}{4K_1^a\lambda_1(\lambda_1^2 - \lambda_2^2)}\sinh(\lambda_1 d/2)\right].
\end{aligned}$$

This yields the following solution of the linearized BVP (4)–(7):

$$\begin{aligned}
\theta(z) &= \frac{a}{12K_1^a}z^3 + \frac{2q_4B_1 + a}{4B_1}z + \frac{q\left[(2\eta - 2\nu)\lambda_1^2 + \nu\lambda_2^2\right]}{2K_1^a\lambda_1\left(\lambda_1^2 - \lambda_2^2\right)}\sinh(\lambda_1 z) + 2q_6\sinh(\lambda_2 z),\\
\delta(z) &= \frac{a}{12K_1^a}z^3 + \frac{2q_4B_1 - a}{4B_1}z + \frac{q\left(\nu\lambda_2^2 - 2\eta\lambda_1^2\right)}{2K_1^a\lambda_1\left(\lambda_1^2 - \lambda_2^2\right)}\sinh(\lambda_1 z) + 2q_7\sinh(\lambda_2 z),\\
u(z) &= a\lambda_p\left[\frac{\cosh(\lambda_1 z)}{\cosh(\lambda_1 d/2)} - 1\right].
\end{aligned}$$

Using Maple, we have verified that the above functions solve equations (5)–(7), satisfy the boundary conditions in (4) and that they are identical with the solution presented in [3, p.1828].

3.2.3 Solutions to the linear problem (4)–(7)

We now rewrite the solution of (4)–(7) as follows:

$$\theta(z) = \frac{a\lambda_p\left[(2\eta - 2\nu)\lambda_1^2 + \nu\lambda_2^2\right]}{2K_1^a\lambda_1(\lambda_1^2 - \lambda_2^2)}\frac{\sinh(\lambda_1 z)}{\cosh(\lambda_1 d/2)} + f(z) - g(z), \tag{27}$$

$$\delta(z) = \frac{a\lambda_p\left(\nu\lambda_2^2 - 2\eta\lambda_1^2\right)}{2K_1^a\lambda_1\left(\lambda_1^2 - \lambda_2^2\right)}\frac{\sinh(\lambda_1 z)}{\cosh(\lambda_1 d/2)} + f(z) + g(z), \tag{28}$$

$$u(z) = a\lambda_p\left[\frac{\cosh(\lambda_1 z)}{\cosh(\lambda_1 d/2)} - 1\right], \tag{29}$$

where

$$\begin{aligned}
f(z) &= \frac{a}{12K_1^a}z^3 + \left[\frac{1}{d}(\delta_0 + \theta_0) - \frac{1}{dK_1^a}\left[\frac{a}{48}d^3 - \frac{a\lambda_p\nu}{\lambda_1}\frac{\sinh(\lambda_1 d/2)}{\cosh(\lambda_1 d/2)}\right]\right]z,\\
g(z) &= \left[\frac{\delta_0 - \theta_0}{2} + \frac{a}{8B_1}d + \frac{a\lambda_p\lambda_1^2(2\eta - \nu)}{2K_1^a\lambda_1(\lambda_1^2 - \lambda_2^2)}\frac{\sinh(\lambda_1 d/2)}{\cosh(\lambda_1 d/2)}\right]\frac{\sinh(\lambda_2 z)}{\sinh(\lambda_2 d/2)} - \frac{a}{4B_1}z.
\end{aligned}$$

These solution functions will be used in this form as starting values for the numerical calculations conducted in Section 4.

Parameter	Typical value
d	10^{-5}
$K_1^a = K_1^n$	5×10^{-12}
B_0	8.95×10^7
B_1	4×10^7
λ_p	10^{-16}
a_1	-0.0060
a_2	-0.0812
a_3	-0.0036
$a4$, τ_1, τ_2	0.0652
a_5	0.0640
κ_1, κ_2,..., κ_6	0.0020
a	-500
θ_0	0.2
δ_0	0.15

Table 1: Typical material parameters specified in [3]

3.3 Calculation with `bvpsuite2.0`

Table 1 contains the values of parameters used from this point forward, see [3, pp.1829-1830].

We use the MATLAB package `bvpsuite2.0` to approximate solutions to the linear BVP (4)–(7). We denote the approximations by $\tilde{\Theta}$, $\tilde{\Delta}$, and $\tilde{U}$. For the simulation, u was scaled by the factor 10^{13} in order to make $\tilde{U} \approx 10^{13}\, u$ an $O(1)$ function, similar in size to $\tilde{\Theta}$ and $\tilde{\Delta}$. Consequently, $\tilde{\Theta} \approx \theta$, $\tilde{\Delta} \approx \delta$, and $\tilde{U} \approx 10^{13}\, u$. The resulting solution plots can be found in Figures 1 and 2. The error estimate, automatically generated by `bvpsuite2.0`, can be found in Figure 3. The exact error of these approximations in relation to the solution functions (27)–(29) is plotted in Figure 4. We used collocation with two Gaussian points and set the absolute and relative tolerance requirements to $Tol_a = Tol_r = 10^{-3}$. We started with a grid of 1000 points and the final grid also contained 1000 points.

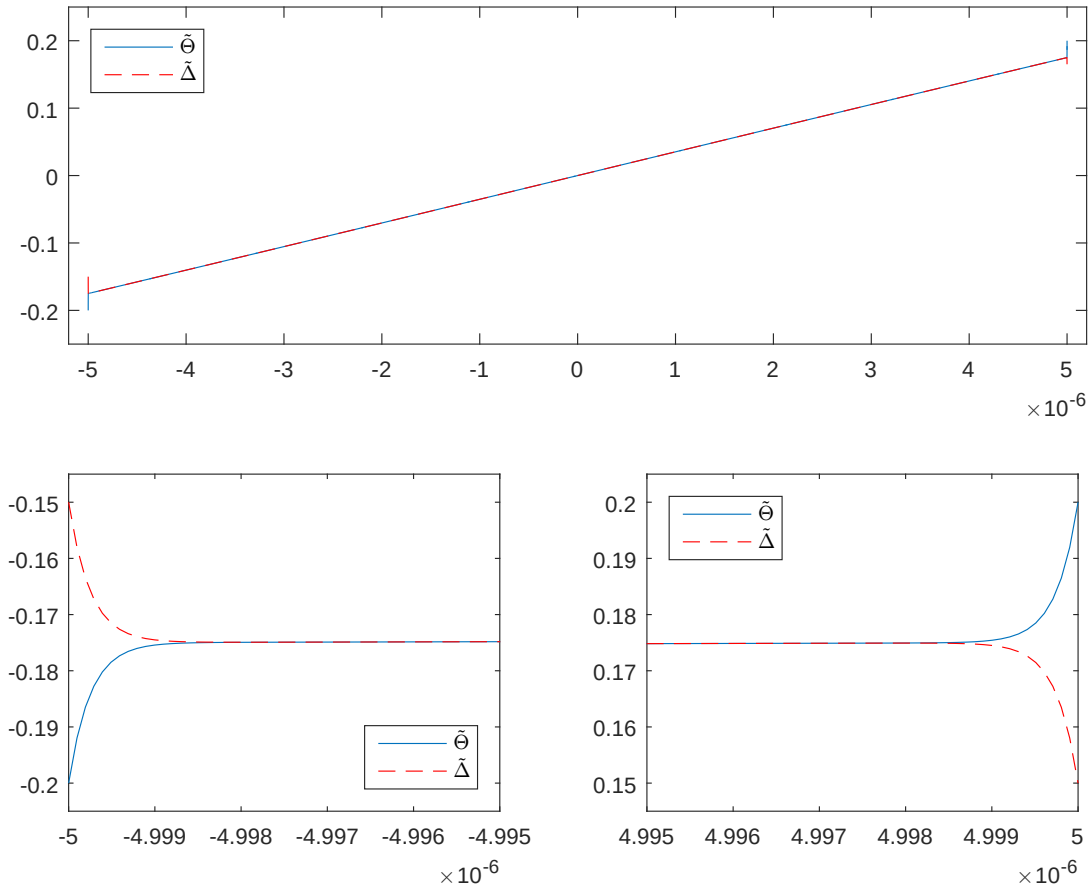

Figure 1: BVP (4)–(7): Approximations $\tilde{\Theta}(z) \approx \theta(z)$ and $\tilde{\Delta}(z) \approx \delta(z)$. In the lower graphs, the areas around the interval boundaries are zoomed in, to enhance the visibility of the solution behaviour.

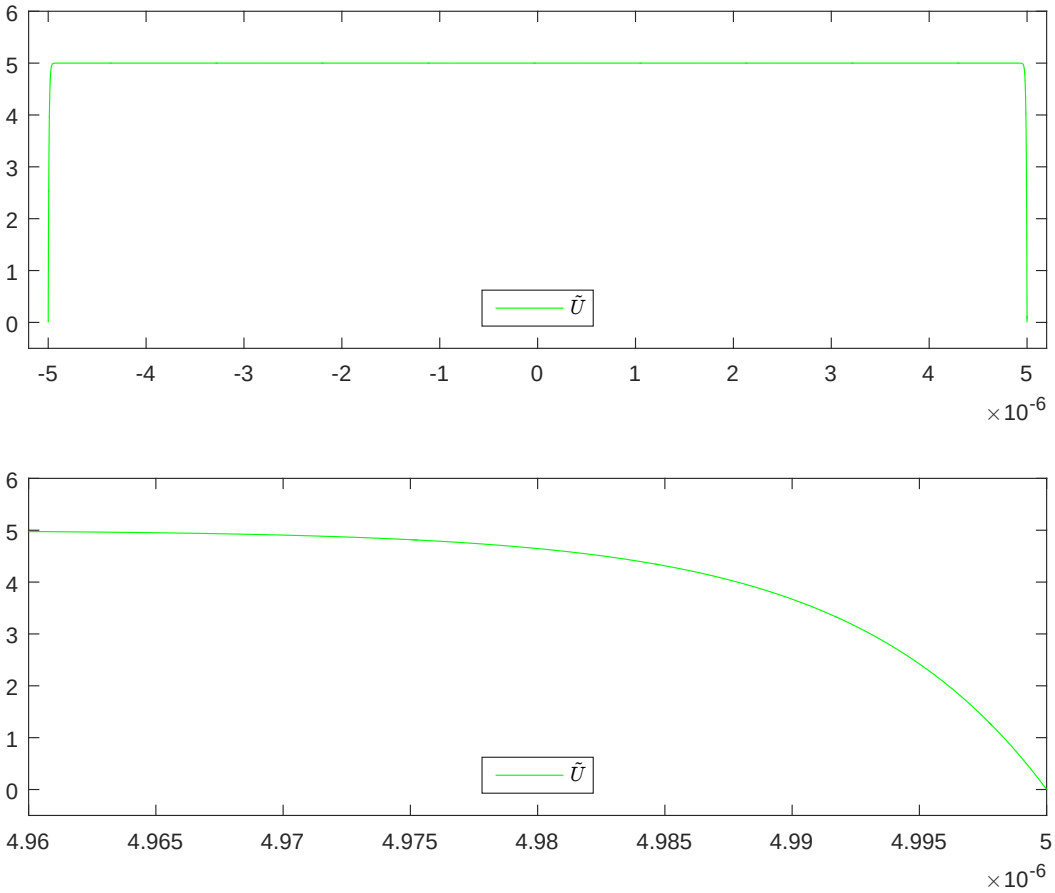

Figure 2: BVP (4)–(7): Approximation $\tilde{U}(z) \approx 10^{13}\, u(z)$. In the lower graph, the area around the right boundary has been zoomed in.

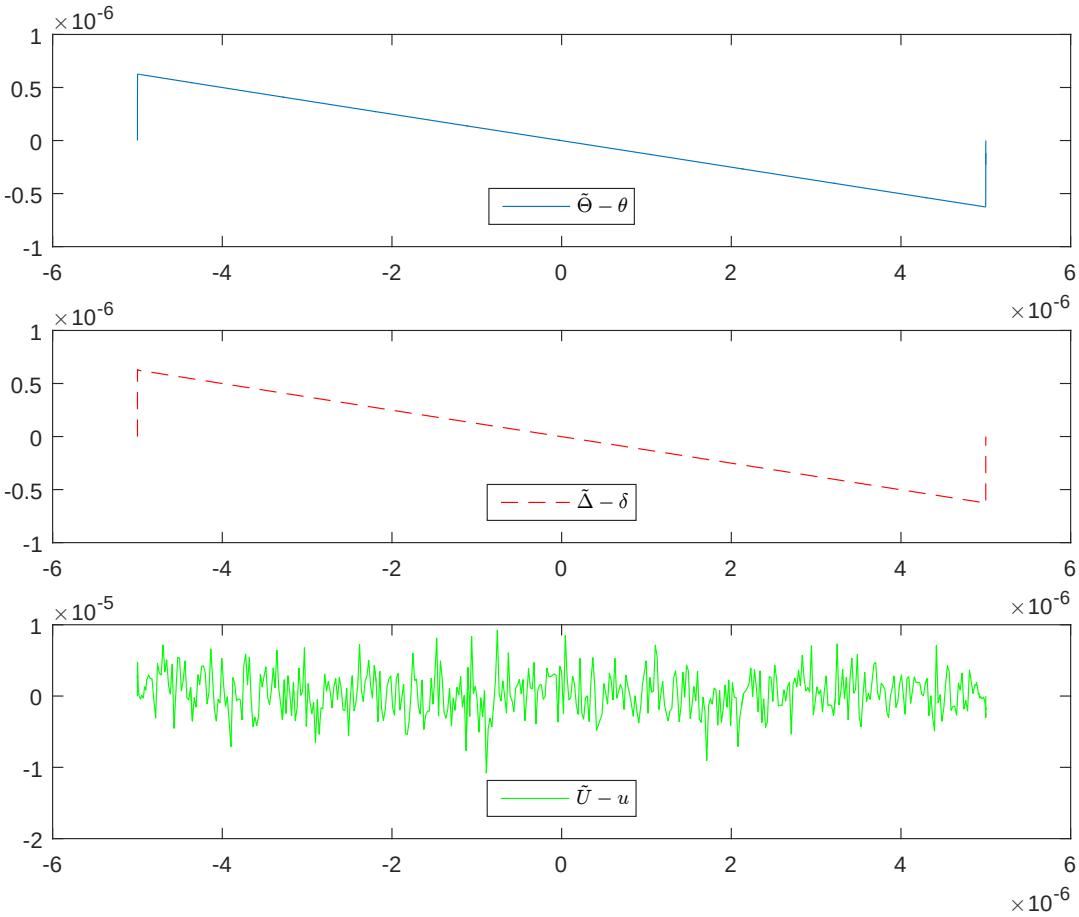

Figure 3: BVP (4)–(7): Absolute global errors of the approximations $\tilde{\Theta}(z) \approx \theta(z)$, $\tilde{\Delta}(z) \approx \delta(z)$ and $\tilde{U}(z) \approx 10^{13}\, u(z)$.

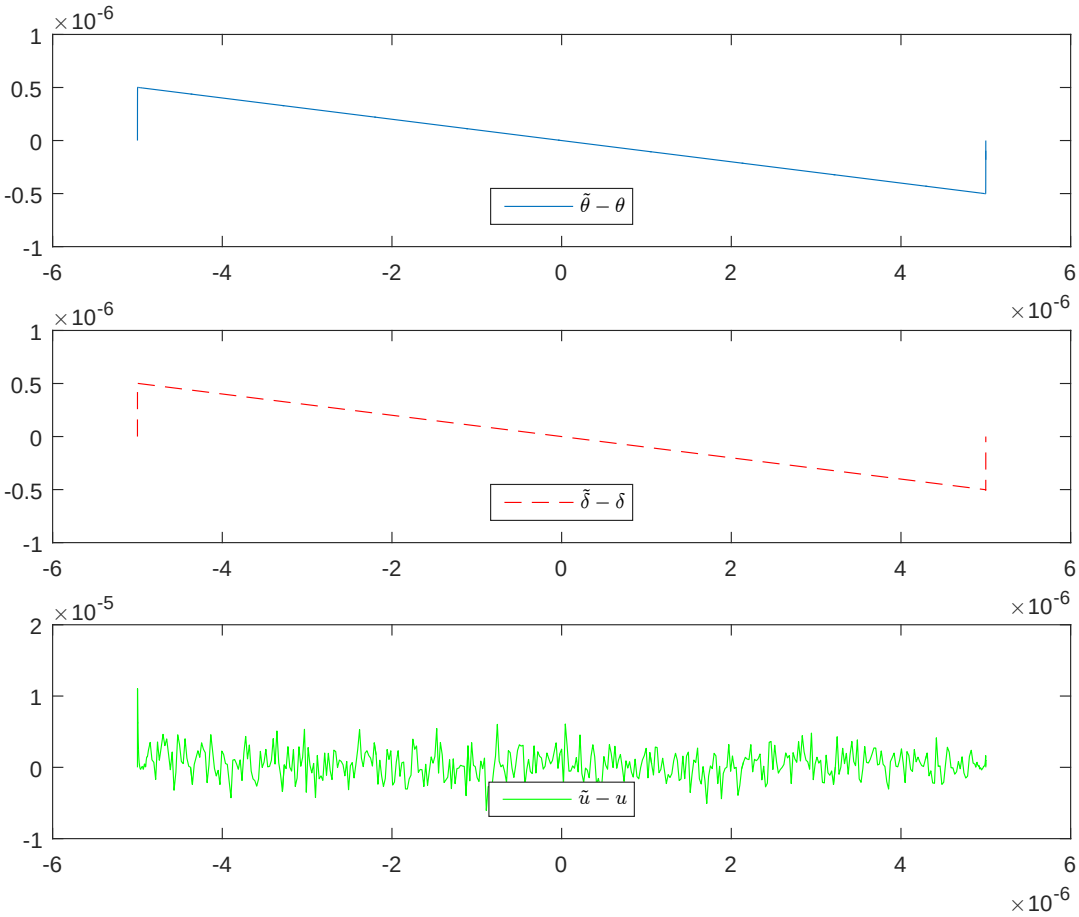

Figure 4: BVP (4)–(7): Exact error of the approximations $\tilde{\Theta}(z) \approx \theta(z)$, $\tilde{\Delta}(z) \approx \delta(z)$ and $\tilde{U}(z) \approx 10^{13}\, u(z)$ compared to the solution functions $\theta(z)$, $\delta(z)$ and $u(z)$ from (27)–(29).

4 Nonlinear problem (1)–(4)

We used the MATLAB package `bvpsuite2.0` to obtain approximations of the solution components to the nonlinear system (1)–(3) and boundary conditions (4). As in the previous section 3.3, we denote the approximations by $\tilde{\Theta} \approx \theta$, $\tilde{\Delta} \approx \delta$, and $\tilde{U} \approx 10^{13}\, u$. The calculations in order to finally set the absolute and relative tolerance requirements to $Tol_a = Tol_r = 10^{-3}$ were carried out in three steps. In each step, the required tolerances were multiplied by a factor of 10^{-1}. In all three steps, we used collocation with one collocation point on a starting grid with 10.000 mesh points.

In the first step, we used the evaluation of the solution functions (27)–(29) at each point from our starting grid as our starting values.

For the second and third step, we used the results of the previous step as starting values.

The results of the numerical calculations for the first step are shown in Figures 5 and 6. In Figure 7, we show the automatically generated error estimate for the (unknown) absolute global error. The required tolerances were set to $Tol_a = Tol_r = 10^{-1}$ in this step. The final grid contained 10.000 points.

Similarly, the results of the numerical calculations for the second step are shown in Figures 8, 9, and 10. The required tolerances were set to $Tol_a = Tol_r = 10^{-2}$ in this step. The final grid contained 14.161 points.

Finally, the results of the numerical calculations for the third step are shown in Figures 11, 12, and 13. The required tolerances were set to $Tol_a = Tol_r = 10^{-3}$ in this step. The final grid contained 40.888 points.

5 Conclusions

We have considered constant pressure-driven 'Poiseuille flow' in a SmA liquid crystal in book-shelf configuration within two parallel plates where both the director and the layer normal are anchored on the plates, but are free to deviate from one and other throughout the layers [2]. The problem is known to have three boundary layers with two of them of the same order but an order of magnitude smaller than the third.

An analytic solution for the linearized equation was developed to act as an initial guess for solving the nonlinear BVP using the MATLAB collocation routine `bvpsuite2.0`. This routine successfully provided the solution of the nonlinear problem with a prescribed accuracy, regardless steep boundary layers, notoriously difficult to resolve.

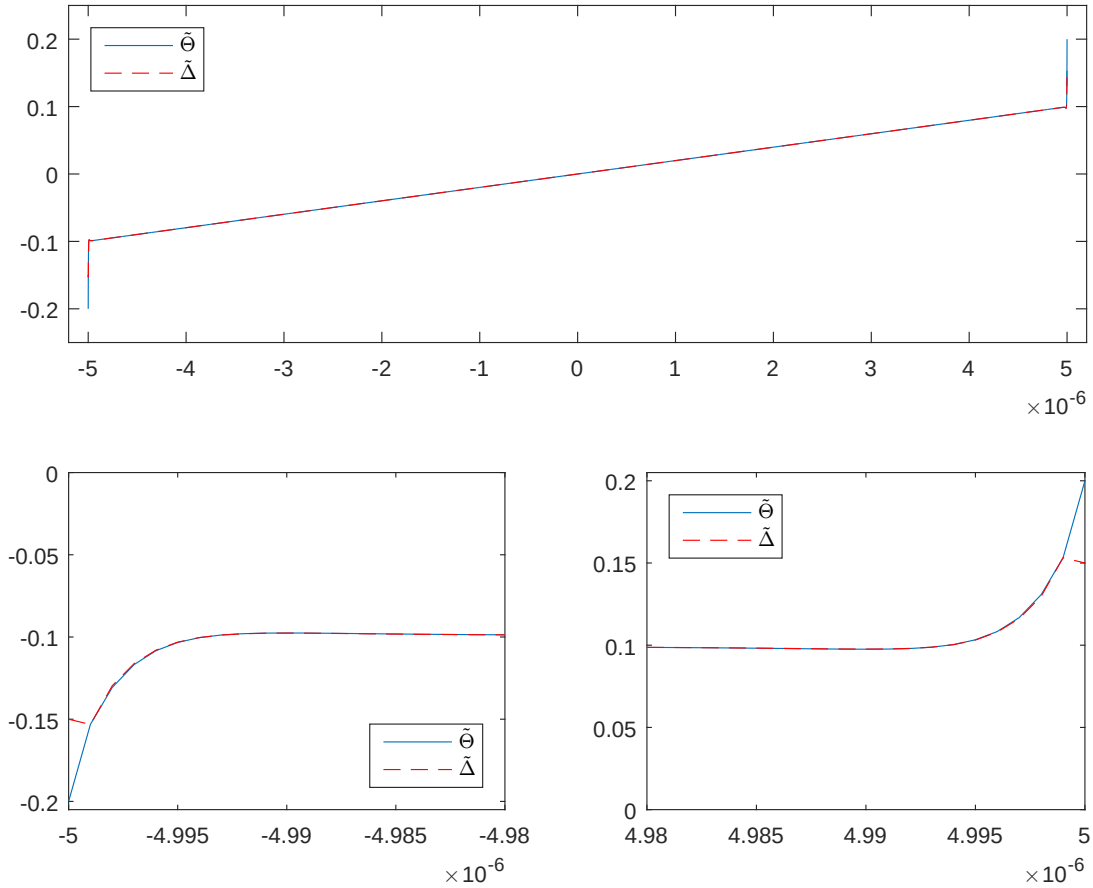

Figure 5: BVP (1)–(4): $Tol_a = Tol_r = 10^{-1}$: Approximations $\tilde{\Theta}(z) \approx \theta(z)$ and $\tilde{\Delta}(z) \approx \delta(z)$. In the lower graphs, the areas around the interval boundaries are zoomed in.

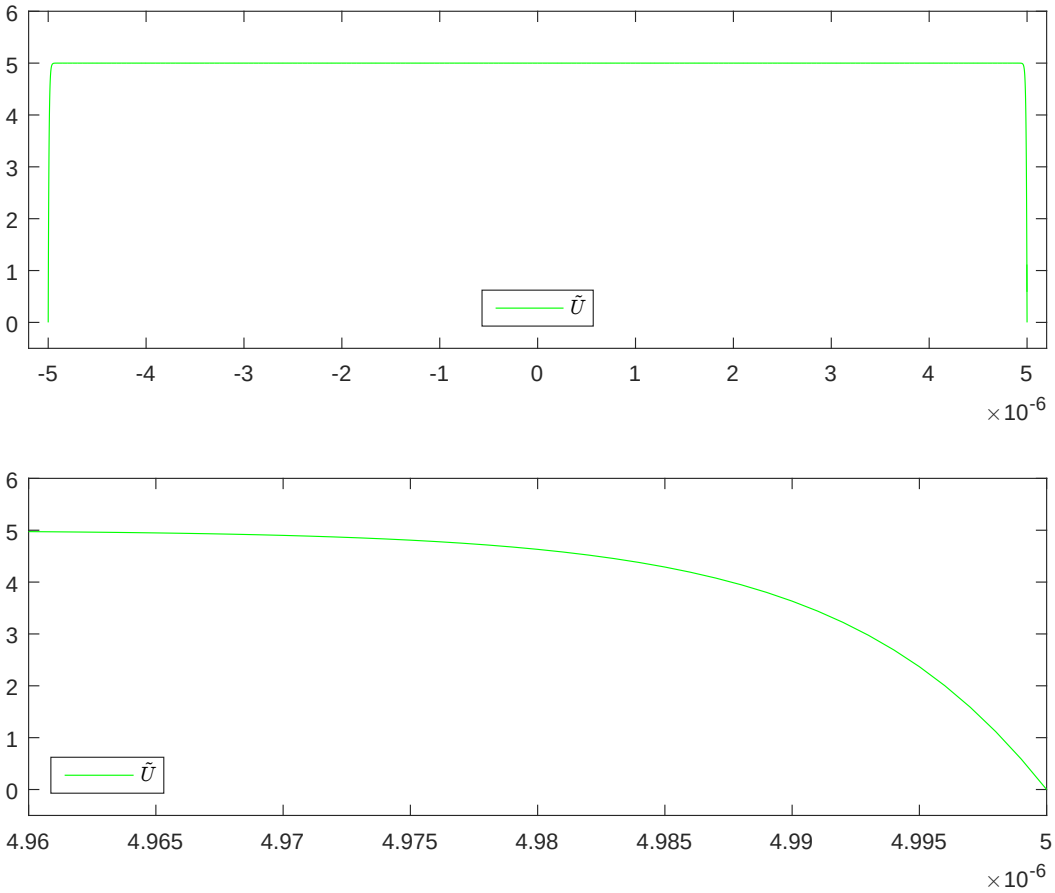

Figure 6: BVP (1)–(4): $Tol_a = Tol_r = 10^{-1}$: Approximation $\tilde{U}(z) \approx 10^{13}\, u(z)$. In the lower graph, the area around the right boundary has been zoomed in.

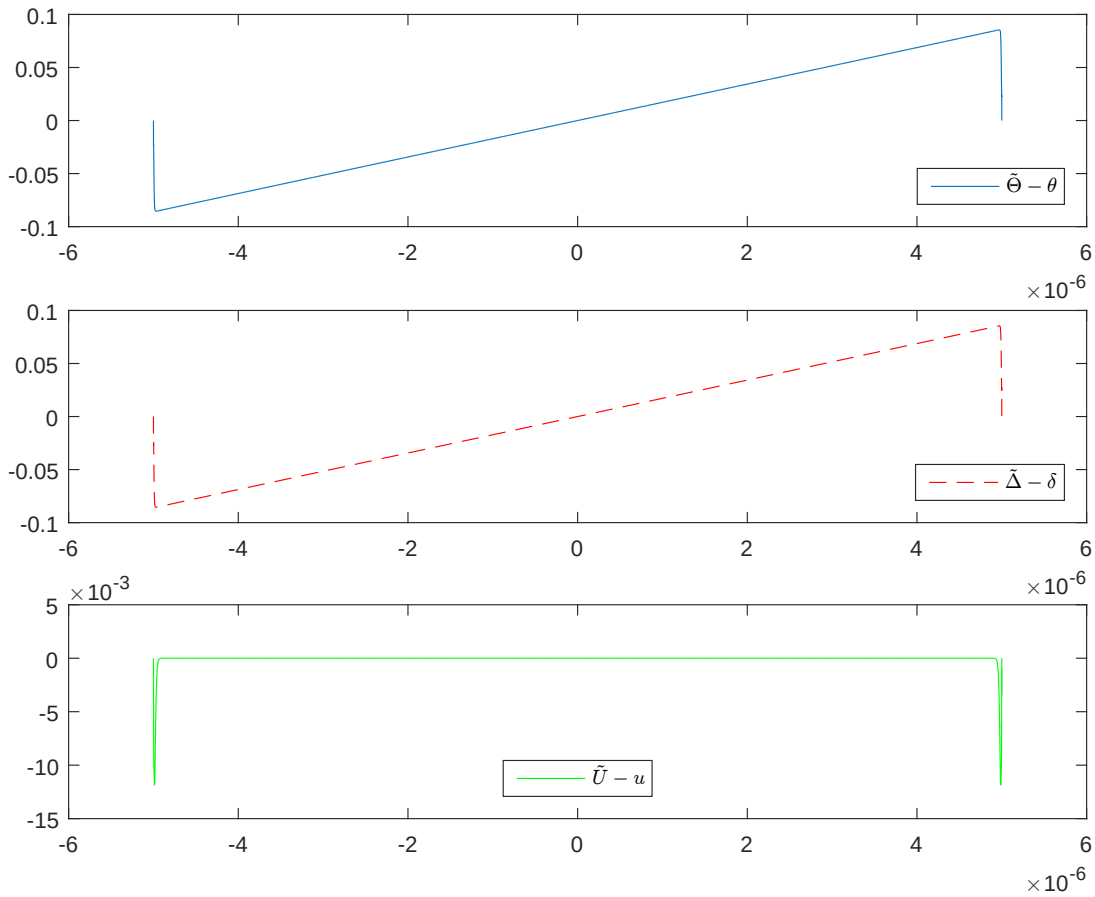

Figure 7: BVP (1)–(4): $Tol_a = Tol_r = 10^{-1}$: Absolute global errors of the approximations $\tilde{\Theta}(z) \approx \theta(z)$, $\tilde{\Delta}(z) \approx \delta(z)$ and $\tilde{U}(z) \approx 10^{13}\, u(z)$.

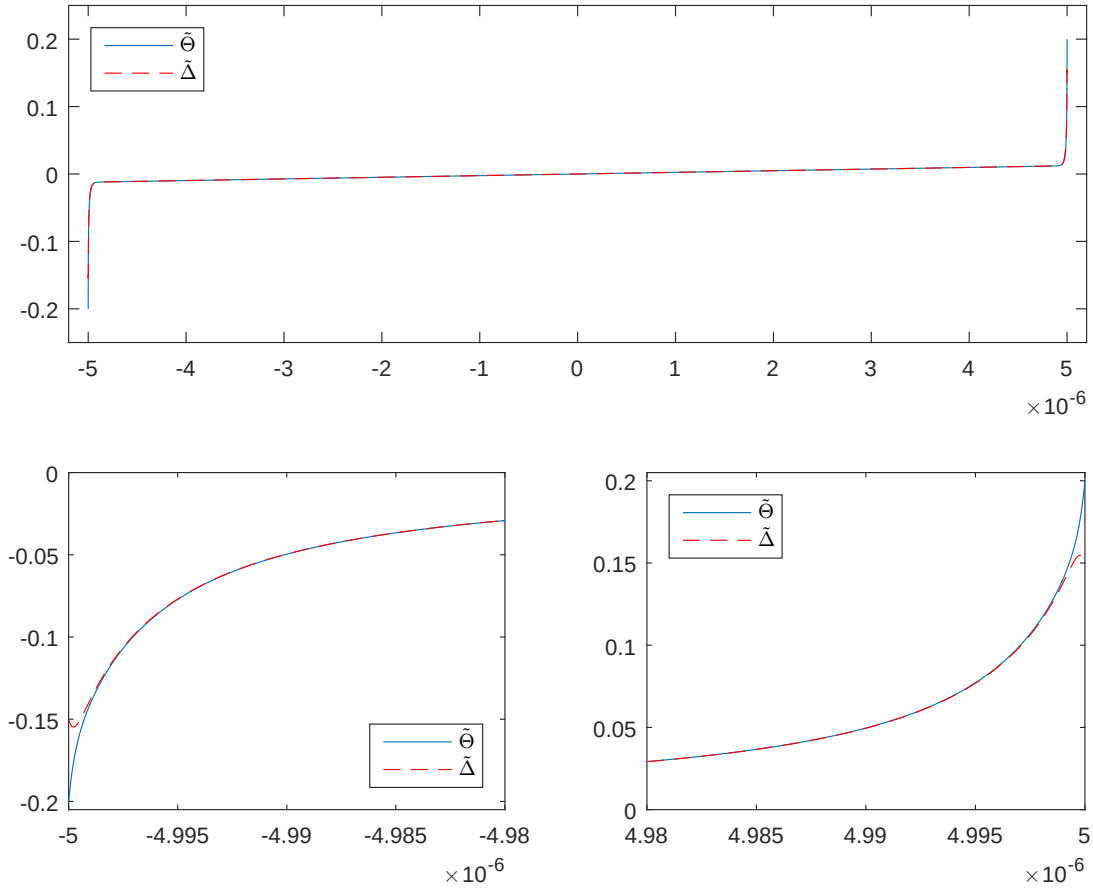

Figure 8: BVP (1)–(4): $Tol_a = Tol_r = 10^{-2}$: Approximations $\tilde{\Theta}(z) \approx \theta(z)$ and $\tilde{\Delta}(z) \approx \delta(z)$. In the lower graphs, the areas around the interval boundaries are zoomed in.

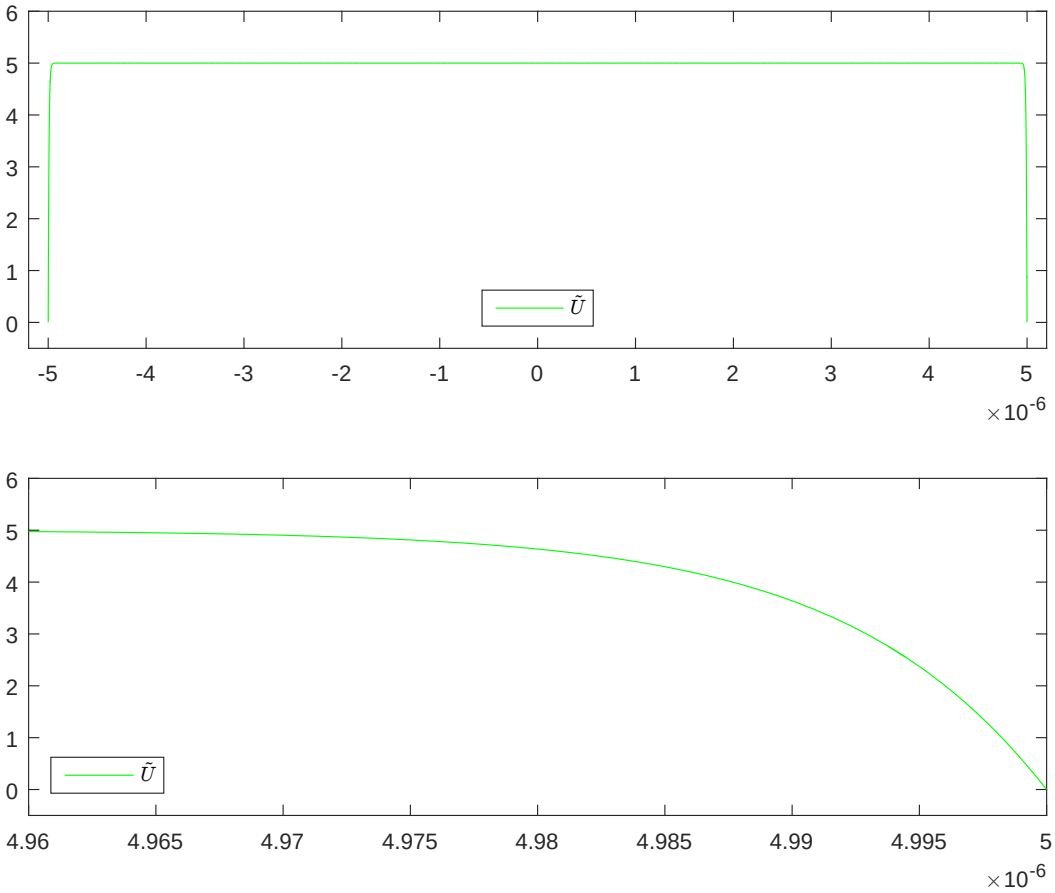

Figure 9: BVP (1)–(4): $Tol_a = Tol_r = 10^{-2}$: Approximation $\tilde{U}(z) \approx 10^{13}\, u(z)$. In the lower graph, the area around the right boundary has been zoomed in.

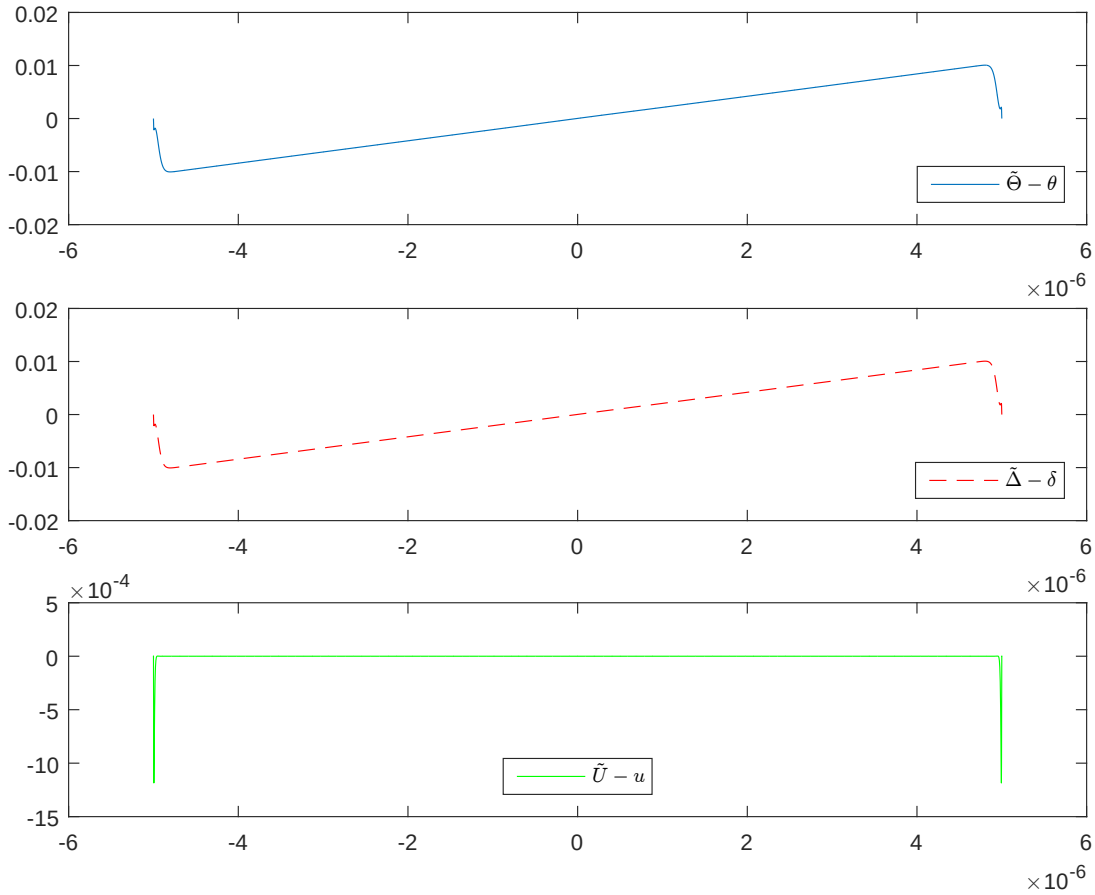

Figure 10: BVP (1)–(4): $Tol_a = Tol_r = 10^{-2}$: Absolute global errors of the approximations $\tilde{\Theta}(z) \approx \theta(z)$, $\tilde{\Delta}(z) \approx \delta(z)$ and $\tilde{U}(z) \approx 10^{13}\, u(z)$.

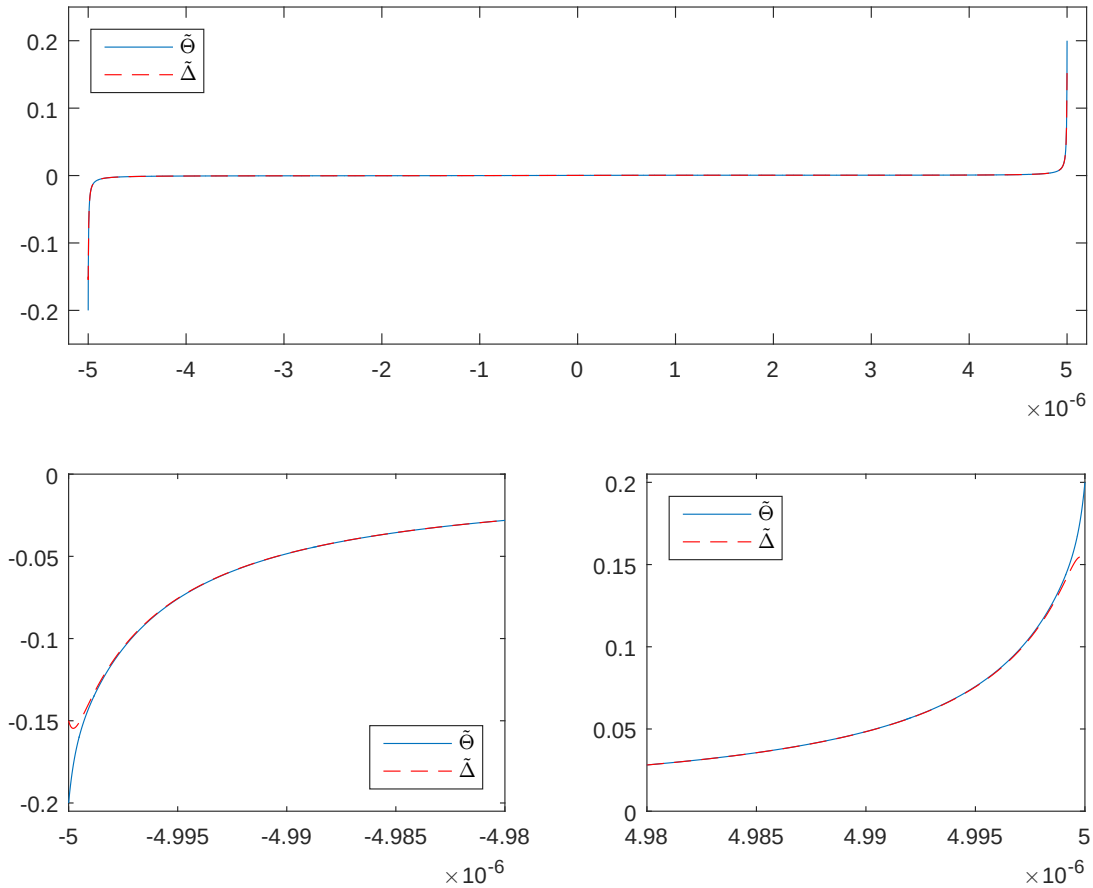

Figure 11: BVP (1)–(4): $Tol_a = Tol_r = 10^{-3}$: Approximations $\tilde{\Theta}(z) \approx \theta(z)$ and $\tilde{\Delta}(z) \approx \delta(z)$. In the lower graphs, the areas around the interval boundaries are zoomed in.

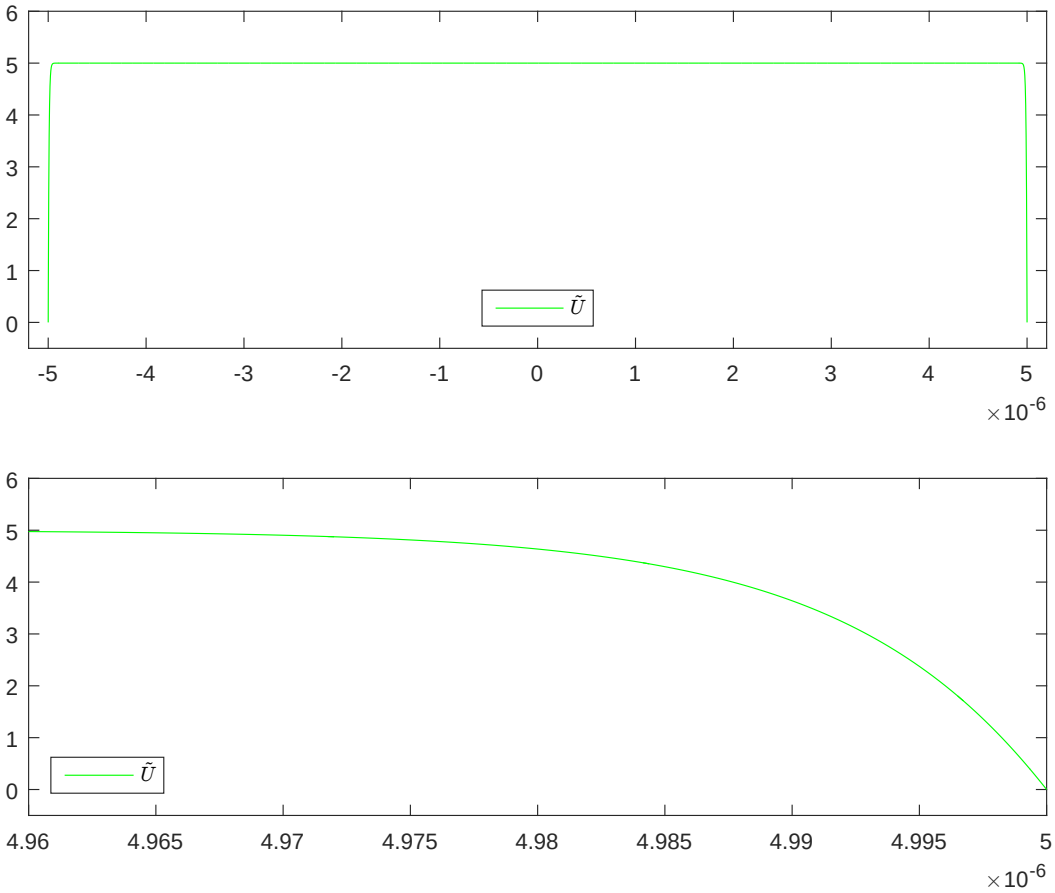

Figure 12: BVP (1)–(4): $Tol_a = Tol_r = 10^{-3}$: Approximation $\tilde{U}(z) \approx 10^{13}\, u(z)$. In the lower graph, the area around the right boundary has been zoomed in.

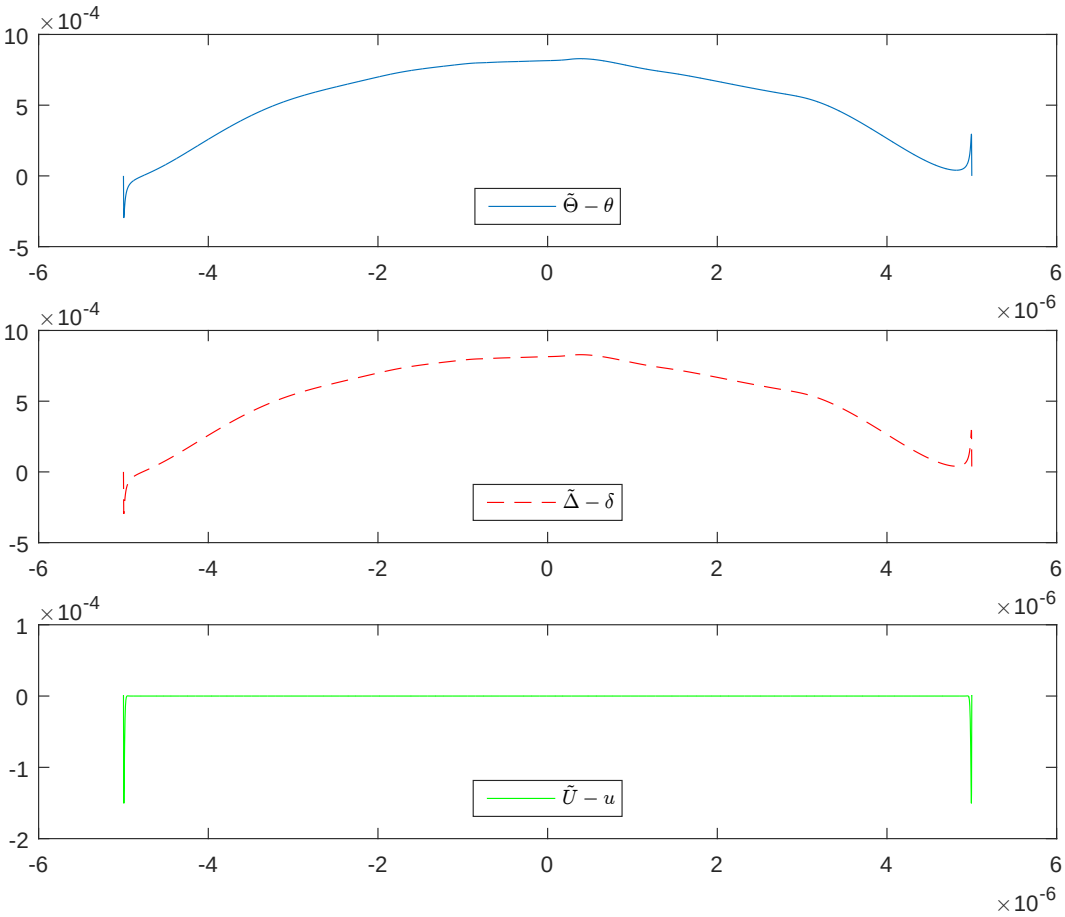

Figure 13: BVP (1)–(4): $Tol_a = Tol_r = 10^{-3}$: Absolute global errors of the approximations $\tilde{\Theta}(z) \approx \theta(z)$, $\tilde{\Delta}(z) \approx \delta(z)$ and $\tilde{U}(z) \approx 10^{13}\, u(z)$.

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