Faster transfer matrix computation for LCD optics

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Abstract

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Introduction

Improved efficiency is desirable when computing transfer matrices because display simulations require solutions of the problem for hundreds of oblique angles of the incident light and numerous wavelengths. A single solution is a small computing problem, but full simulations may be time-consuming [2,5].

The 4×4 model for optics in anisotropic media is a linear system of ordinary differential equations characterized by a 4×4 matrix. Berreman applied this model to display cells [1] having an optically varying liquid-crystal layer of thickness d (about 5 μm). His solution method is to approximate the variation of optical anisotropy with depth in the liquid-crystal using a stack of individually homogeneous anisotropic layers. The composite of the transfer matrices for these layers approaches the true transfer matrix for the medium, as more and thinner layers are used.

Two approaches to computing transfer matrices for the homogeneous layers, the eigenvector method [9], and the Cayley-Hamilton method [10], are widely used. A third approach, the Newton-Putzer method, is introduced here. This new approach proves to compute transfer matrices more rapidly than do the previous methods.

General Method

The objectives of the 4×4 model are the fields $\mathbf{E}$ and $\mathbf{H}$ of Maxwell's equations. The problem depends upon the direction of the obliquely incident light represented by its unit wave propagation vector $\mathbf{q} = (c_{\text{ext}}/\omega)\mathbf{k}$, where c_{ext} is the group velocity in the external medium. The other important problem datum, the 3×3 relative anisotropy tensor $\boldsymbol{\varepsilon}(z)$, varies with depth z in the liquid-crystal, but is constant in the lateral x and y directions. The last input, polarization of the incident wave, enters only the boundary or initial conditions of the problem. The field functions that result inside the liquid-crystal oscillate with varying frequencies that are proportional to the dimensionless wave number $k_0 = \omega\, d/c_{\text{ext}}$. For visible light in a display cell of typical thickness, k_0 has a value in the range of 50 to 500 radians.

When the lateral dimensions of a display pixel are large compared to its thickness, Maxwell's curl equations, along with the constitutive relation $\mathbf{D}(\mathbf{r},t) = \boldsymbol{\varepsilon}(z)\mathbf{E}(\mathbf{r},t)$, are solved by hypothesizing solution functions that are the real parts of

$$(1)\qquad \mathbf{E}(\mathbf{r},t) = \hat{\mathbf{E}}(z)\exp[ik_0(q_1 x + q_2 y - t)]$$
$$\mathbf{H}(\mathbf{r},t) = \hat{\mathbf{H}}(z)\exp[ik_0(q_1 x + q_2 y - t)],$$

where the q_l are the components of the wave vector $\mathbf{q}$, and $\mathbf{r} = (x, y, z)$ and t are non-dimensional coordinates proportional to the usual space and time coordinates via the factors $1/d$ and c_{ext}/d respectively.

The Maxwell curl formulas yield a system of o.d.e.'s for the target functions $\hat{\mathbf{E}}(z)$ and $\hat{\mathbf{H}}(z)$ because time derivatives and spatial derivatives in x and y give algebraic relations. When multiplied with the exponentials as in (1), these functions mathematically satisfy the Maxwell equations.

The 4×4 model targets only the transverse field components $\boldsymbol{\psi}(z) = (\hat{E}_1(z), \hat{H}_2(z), \hat{E}_2(z), -\hat{H}_1(z))$, and the system of ordinary differential equations that defines these functions is summarized:

$$(2)\qquad \boldsymbol{\psi}'(z) = ik_0\boldsymbol{\Delta}(z)\boldsymbol{\psi}(z),$$

where the 4×4 matrix $\boldsymbol{\Delta}(z)$ consists of four 2×2 blocks. Specifically, $\boldsymbol{\Delta} = \lfloor \boldsymbol{\Delta}_{ij} \rfloor$ for $i, j \in \{1,2\}$ with the $\boldsymbol{\Delta}_{ij}$ taking [6] the forms

$$\begin{bmatrix} -\dfrac{\varepsilon_{3j}}{\varepsilon_{33}} q_i & \delta_i^j - \dfrac{1}{\varepsilon_{33}} q_i q_j \\ \left(\varepsilon_{ij} - \dfrac{\varepsilon_{i3}\varepsilon_{3j}}{\varepsilon_{33}}\right) + (-1)^{i+j-1} q_{m(i)} q_{m(j)} & -\dfrac{\varepsilon_{i3}}{\varepsilon_{33}} q_j \end{bmatrix},$$

where δ_i^j is the Kronecker delta, ε_{kl} are the entries of the anisotropy tensor, and the evaluates of m are $m(1) = 2$ and $m(2) = 1$. The matrix $\boldsymbol{\Delta}(z)$ varies with normalized depth $0 \le z \le 1$ inside the liquid-crystal layer because the entries ε_{kl} of the tensor $\boldsymbol{\varepsilon}(z)$ vary with depth. The q_l are fixed constants.

Depending on the physics of the device, the 4×4 model may be stated either as an initial value or a boundary value problem. In any case, the continuous 4×4 transfer matrix function $\mathbf{P}(z)$ serves as a basis [2] for solutions to the system (2), and it is a fundamental solution matrix for the system. The existence of the transfer matrix is guaranteed in terms of Picard's convergent series of iterated integrals, though this convergence is rather slow.

Exact solutions to the system (2) are known only for special cases [4], and so approximate numerical solutions are often used. A high order Runge-Kutta method may be applied to the computations, though this approach is also slow to converge in that its error per step is afflicted with high powers of the problem parameter k_0, necessitating approximately ten steps per wavelength merely to attain a relative error of 0.01 in the computed solution. The best numerical approach is to approximate the liquid-crystal using a stack of N homogeneous anisotropic layers. For two digit accuracy in the solution, it usually suffices to set N high enough to have each layer be about one wavelength thick.

The layers need not all be the same thickness, but for one lying between $z = z_{j-1}$ and $z = z_j$ and having thickness h_j, it's important to use the anisotropy $\boldsymbol{\varepsilon}(z_{j-1/2})$ at the midpoint $z = z_{j-1/2}$ of the interval as the tensor for the entire layer. Also note that the matrix

$$(3) \qquad \boldsymbol{\Delta}_{(j)} = \boldsymbol{\Delta}(z_{j-1/2})$$

derived from $\boldsymbol{\varepsilon}(z_{j-1/2})$ is always diagonalizable, and admits the decomposition

$$(4) \qquad \boldsymbol{\Delta}_{(j)} = \mathbf{V}_{(j)} \boldsymbol{\Lambda}_{(j)} \mathbf{V}_{(j)}^{-1},$$

where $\mathbf{V}_{(j)}$ is the matrix of eigenvectors and $\boldsymbol{\Lambda}_{(j)}$ is the diagonal eigenvalue matrix.

The layers in the stack are anisotropic, but each is also homogeneous. Because of this, the transfer matrices are matrix exponentials that are defined as convergent infinite sums in powers of $\boldsymbol{\Delta}_{(j)}$, and for the jth layer, the transfer matrix is exactly

$$(5) \qquad \mathbf{P}_{\Delta(j)}(z) = \exp\left[ik_0 (z - z_{j-1}) \boldsymbol{\Delta}_{(j)}\right].$$

The matrix exponential is the correct transfer matrix because its derivative equals $ik_0 \boldsymbol{\Delta}_{(j)}$ multiplied by the exponential. When evaluating one of the single interval transfer matrices for the full width of the layer, we'll abbreviate it with the notation $\mathbf{P}_{\Delta(j)} = \mathbf{P}_{\Delta(j)}(z_j)$, and a composite numerical transfer matrix for the entire system of differential equations is the product

$$(6) \qquad \mathbf{P}_{\Delta(N)} \mathbf{P}_{\Delta(N-1)} \cdots \mathbf{P}_{\Delta(2)} \mathbf{P}_{\Delta(1)}.$$

Numerical Approaches

Each step requires information about the approximate medium in the layer, and a computation that gives the exact transfer matrix for the layer. The eigenvector method, the Cayley-Hamilton method, and the Newton-Putzer method all compute this transfer matrix.

For the jth step (layer), all three methods require either exact or very accurate eigenvalues for the matrix $\boldsymbol{\Delta}_{(j)}$. When the liquid-crystal is uniaxial, the four eigenvalues [10] are:

$$\lambda_{1(j)} = -\frac{\bar{\varepsilon}_{13}}{\bar{\varepsilon}_{33}} \chi + \left[\left(\frac{\bar{\varepsilon}_{13}}{\bar{\varepsilon}_{33}} \chi \right)^2 + \frac{\varepsilon_\perp \varepsilon_= - \bar{\varepsilon}_{11} \chi^2}{\bar{\varepsilon}_{33}} \right]^{1/2},$$

$$\lambda_{3(j)} = -\frac{\bar{\varepsilon}_{13}}{\bar{\varepsilon}_{33}} \chi - \left[\left(\frac{\bar{\varepsilon}_{13}}{\bar{\varepsilon}_{33}} \chi \right)^2 + \frac{\varepsilon_\perp \varepsilon_= - \bar{\varepsilon}_{11} \chi^2}{\bar{\varepsilon}_{33}} \right]^{1/2},$$

$$\lambda_{2(j)} = \left(\varepsilon_\perp - \chi^2\right)^{1/2}, \qquad \lambda_{4(j)} = -\left(\varepsilon_\perp - \chi^2\right)^{1/2},$$

where $\varepsilon_\perp$ and $\varepsilon_=$ are the ordinary and extraordinary dielectrics for the l.c., χ is the length of $(q_1, q_2, 0)$, and the entries $\bar{\varepsilon}_{kl}$ are those of a version of the tensor $\boldsymbol{\varepsilon}(z_{j-1/2})$ where the reference frame has been rotated to have $\mathbf{q}$ occur in the $xz-$plane. The transfer matrix for the jth layer can be developed by any one of the three formulas:

$$(7) \qquad \mathbf{P}_{\Delta(j)} = \mathbf{V}_{(j)} e^{ik_o h_j \boldsymbol{\Lambda}_{(j)}} \mathbf{V}_{(j)}^{-1}$$

eigenvector method,

$$(8) \qquad \mathbf{P}_{\Delta(j)} = c_1(h_j)\mathbf{I} + c_2(h_j)\boldsymbol{\Delta}_{(j)} + c_3(h_j)\boldsymbol{\Delta}_{(j)}^2 + c_4(h_j)\boldsymbol{\Delta}_{(j)}^3$$

Cayley – Hamilton method,

$$(9) \qquad \begin{aligned} \mathbf{P}_{\Delta(j)} = {} & r_1(h_j)\mathbf{I} + ik_0 r_2(h_j)\left[\boldsymbol{\Delta}_{(j)} - \lambda_{1(j)}\mathbf{I}\right] \\ & + (ik_0)^2 r_3(h_j)\left[\boldsymbol{\Delta}_{(j)} - \lambda_{2(j)}\mathbf{I}\right]\left[\boldsymbol{\Delta}_{(j)} - \lambda_{1(j)}\mathbf{I}\right] \\ & + (ik_0)^3 r_4(h_j)\left[\boldsymbol{\Delta}_{(j)} - \lambda_{3(j)}\mathbf{I}\right]\left[\boldsymbol{\Delta}_{(j)} - \lambda_{2(j)}\mathbf{I}\right] \\ & \cdot \left[\boldsymbol{\Delta}_{(j)} - \lambda_{1(j)}\mathbf{I}\right] \end{aligned}$$

Newton – Putzer method,

where the coefficients $c_i(h_j)$ or $r_i(h_j)$ are found by solving simple algebraic systems.

The eigenvector method gives a transfer matrix for the *j*th layer because the matrix exponential can be stated in terms of the eigenvectors for $\mathbf{\Delta}_{(j)}$. Formulas for these eigenvectors appear in a paper by Eidner [3]. The derivative of (7) is

$$\frac{d}{dz}\left\{\mathbf{V}_{(j)}e^{ik_0(z-z_{j-1})\mathbf{\Lambda}_{(j)}}\mathbf{V}_{(j)}^{-1}\right\} = \mathbf{V}_{(j)}ik_0\mathbf{\Lambda}_{(j)}e^{ik_0(z-z_{j-1})\mathbf{\Lambda}_{(j)}}\mathbf{V}_{(j)}^{-1} = \mathbf{V}_{(j)}ik_0\mathbf{\Lambda}_{(j)}\mathbf{V}_{(j)}^{-1} \cdot \mathbf{V}_{(j)}e^{ik_0(z-z_{j-1})\mathbf{\Lambda}_{(j)}}\mathbf{V}_{(j)}^{-1} = ik_0\mathbf{\Delta}_{(j)}\exp\left[ik_0(z-z_{j-1})\mathbf{\Delta}_{(j)}\right],$$

so the differential equation (2) is satisfied.

The formula (8) gives the same transfer matrix because its coefficients are solutions of the system

$$(10)\quad \begin{bmatrix} 1 & \lambda_{1(j)} & \lambda_{1(j)}^2 & \lambda_{1(j)}^3 \\ 1 & \lambda_{2(j)} & \lambda_{2(j)}^2 & \lambda_{2(j)}^3 \\ 1 & \lambda_{3(j)} & \lambda_{3(j)}^2 & \lambda_{3(j)}^3 \\ 1 & \lambda_{4(j)} & \lambda_{4(j)}^2 & \lambda_{4(j)}^3 \end{bmatrix}\begin{bmatrix} c_1(h_j) \\ c_2(h_j) \\ c_3(h_j) \\ c_4(h_j) \end{bmatrix} = \begin{bmatrix} e^{ik_0h_j\lambda_{1(j)}} \\ e^{ik_0h_h\lambda_{2(j)}} \\ e^{ik_0h_j\lambda_{3(j)}} \\ e^{ik_0h_j\lambda_{4(j)}} \end{bmatrix}.$$

The Cayley-Hamilton theorem of matrix algebra asserts that the fourth degree characteristic polynomial for the matrix $\mathbf{\Delta}_{(j)}$, when evaluated at that matrix, gives the identically zero matrix. This means that $\mathbf{\Delta}_{(j)}^4$ can be written as a polynomial in $\mathbf{I}, \mathbf{\Delta}_{(j)}, \mathbf{\Delta}_{(j)}^{\mathbf{2}}$ and $\mathbf{\Delta}_{(j)}^3$, and so in addition, can higher powers of the matrix. Even a convergent infinite sum, like the matrix exponential, can be stated:

$$(11)\quad \exp\left[ik_0h_j\mathbf{\Delta}_{(j)}\right] = c_1(h_j)\mathbf{I} + c_2(h_j)\mathbf{\Delta}_{(j)} + c_3(h_j)\mathbf{\Delta}_{(j)}^2 + c_4(h_j)\mathbf{\Delta}_{(j)}^3.$$

Note that pre- and post-multiplying the sum (11) by the eigenvector matrices $\mathbf{V}_{(j)}^{-1}$ and $\mathbf{V}_{(j)}$ gives

$$(12)\quad \exp\left[ik_0h_j\mathbf{\Lambda}_{(j)}\right] = c_1(h_j)\mathbf{I} + c_2(h_j)\mathbf{\Lambda}_{(j)} + c_3(h_j)\mathbf{\Lambda}_{(j)}^2 + c_4(h_j)\mathbf{\Lambda}_{(j)}^3.$$

The twelve off-diagonal equations of the system (12) have the form zero equals zero. The four equations on the diagonal of (12) comprise the system (10) for the $c_i(h_j)$.

The Newton-Putzer method (9) also yields a transfer matrix for the *j*th layer because the coefficients r_i as functions of h_j are solutions to the following system of differential equations with constant coefficients:

$$(13)\quad \begin{aligned} r_1'(t) &= ik_0\lambda_{1(j)}r_1(t), & r_1(0) &= 1 \\ r_2'(t) &= ik_0\lambda_{2(j)}r_2(t) + r_1(t), & r_2(0) &= 0 \\ r_3'(t) &= ik_0\lambda_{3(j)}r_3(t) + r_2(t), & r_3(0) &= 0 \\ r_4'(t) &= ik_0\lambda_{4(j)}r_4(t) + r_3(t), & r_4(0) &= 0 \end{aligned}$$

where the independent variable $t = z - z_{j-1}$. This method has been adapted for use in the transfer matrix problem from ideas described in [7]. The functions r_i were described earlier as solutions to an algebraic system because they can be computed via a tableau of divided differences.

To prove that the Newton-Putzer expansion is the transfer matrix, the divided differences are not required, and we use instead the definitions of the r_i as solutions of the initial value problem (13). Let

$$\mathbf{F}_{1(j)} = ik_0\left[\mathbf{\Delta}_{(j)} - \lambda_{1(j)}\mathbf{I}\right]$$
$$\mathbf{F}_{2(j)} = (ik_0)^2\left[\mathbf{\Delta}_{(j)} - \lambda_{2(j)}\mathbf{I}\right]\left[\mathbf{\Delta}_{(j)} - \lambda_{1(j)}\mathbf{I}\right]$$
$$\mathbf{F}_{3(j)} = (ik_0)^3\left[\mathbf{\Delta}_{(j)} - \lambda_{3(j)}\mathbf{I}\right]\left[\mathbf{\Delta}_{(j)} - \lambda_{2(j)}\mathbf{I}\right] \cdot \left[\mathbf{\Delta}_{(j)} - \lambda_{1(j)}\mathbf{I}\right]$$
$$\mathbf{F}_{4(j)} = (ik_0)^4\left[\mathbf{\Delta}_{(j)} - \lambda_{4(j)}\mathbf{I}\right]\left[\mathbf{\Delta}_{(j)} - \lambda_{3(j)}\mathbf{I}\right] \cdot \left[\mathbf{\Delta}_{(j)} - \lambda_{2(j)}\mathbf{I}\right]\left[\mathbf{\Delta}_{(j)} - \lambda_{1(j)}\mathbf{I}\right]$$

and define a 4×4 matrix function via the expansion

$$\mathbf{F}_{(j)}(t) = r_1(t)\mathbf{I} + r_2(t)\mathbf{F}_{1(j)} + r_3(t)\mathbf{F}_{2(j)} + r_4(t)\mathbf{F}_{3(j)}.$$

Observe that the derivative for $\mathbf{F}_{(j)}(t)$ is

$$\begin{aligned} \mathbf{F}_{(j)}'(t) &= r_1'(t)\mathbf{I} + r_2'(t)\mathbf{F}_{1(j)} + r_3'(t)\mathbf{F}_{2(j)} + r_4'(t)\mathbf{F}_{3(j)} \\ &= ik_0\lambda_{1(j)}r_1(t)\mathbf{I} \\ &\quad + \left[ik_0\lambda_{2(j)}r_2(t) + r_1(t)\right]\mathbf{F}_{1(j)} \\ &\quad + \left[ik_0\lambda_{3(j)}r_3(t) + r_2(t)\right]\mathbf{F}_{2(j)} \\ &\quad + \left[ik_0\lambda_{4(j)}r_4(t) + r_3(t)\right]\mathbf{F}_{3(j)}, \end{aligned}$$

then collecting terms for $r_1(t), r_2(t), r_3(t), r_4(t)$, and using $\mathbf{F}_{i+1(j)} = ik_0\left[\mathbf{\Delta}_{(j)} - \lambda_{i+1(j)}\mathbf{I}\right]\mathbf{F}_{i(j)}$, we obtain

$$(14)\quad \mathbf{F}_{(j)}'(t) = ik_0r_1(t)\mathbf{\Delta}_{(j)} + ik_0r_2(t)\mathbf{\Delta}_{(j)}\mathbf{F}_{1(j)} + ik_0r_3(t)\mathbf{\Delta}_{(j)}\mathbf{F}_{2(j)} + ik_0r_4(t)\lambda_{4(j)}\mathbf{F}_{3(j)}.$$

Adding and subtracting the term $ik_0 r_4(t)\boldsymbol{\Delta}_{(j)}\mathbf{F}_{3(j)}$ in (14) now makes

$$\mathbf{F}'_{(j)}(t) = ik_0\boldsymbol{\Delta}_{(j)}\mathbf{F}_{(j)}(t) - ik_0 r_4(t)\left[\boldsymbol{\Delta}_{(j)} - \lambda_{4(j)}\mathbf{I}\right]\mathbf{F}_{3(j)}(t).$$

Since $\mathbf{F}_{4(j)} = ik_0\left[\boldsymbol{\Delta}_{(j)} - \lambda_{4(j)}\mathbf{I}\right]\mathbf{F}_{3(j)} = \mathbf{0}$ by the Cayley-Hamilton theorem, we've proved that

$$\mathbf{F}'_{(j)}(t) = ik_0\boldsymbol{\Delta}_{(j)}\mathbf{F}_{(j)}(t),$$

so the Newton-Putzer formula (9) is exactly the transfer matrix for the *j*th liquid-crystal layer.

Computational Speed

Evidence that the Newton-Putzer method is faster than the other methods is presented in Figure 1 for a simple TN cell with $k_0 = 100$ for light incident at 30 degrees. Computation times were observed on an HP 9000/782 computer with a 500 MHz processor running

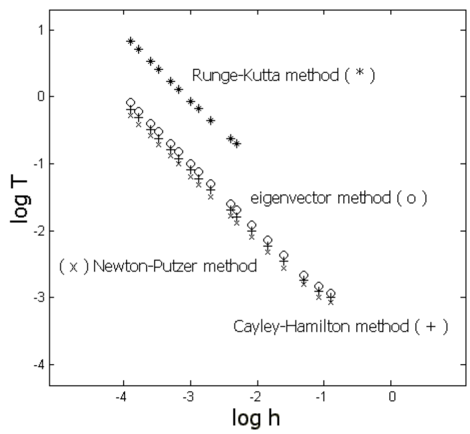

Figure 1. Timings versus stepsize.

Fortran90. The timings for the three transfer matrix methods, as well as a fifth order Runge-Kutta method, are graphed as functions of uniform layer thickness h (the length of a step). The intercepts for the plots provide constants C in the computational complexity estimates $T \cong C/h$. Table 1 presents the estimates of C (in seconds per step).

The transfer matrix methods are faster than the Runge-Kutta method by approximately a factor of ten because the error term in Runge-Kutta is $O\left(k_0(k_0 h)^5\right)$ [8]. The corresponding error term for the transfer matrix methods is $O\left(k_0 h^2\right)$ as $h \to 0$.

The better performance of the Newton-Putzer and Cayley-Hamilton methods as compared to the eigenvector method is because these do not need the matrix

method	s / step	ratio
Newton-Putzer	6.892×10^{-5}	0.66
Cayley-Hamilton	8.455×10^{-5}	0.81
eigenvector	1.050×10^{-4}	1.00
Runge-Kutta	8.711×10^{-4}	8.30

Table 1. Estimated *C* from line intercepts.

eigenvectors in each layer [10]. The Newton-Putzer method is computationally cheaper than the Cayley-Hamilton method because its coefficients can be computed using the Newtonian divided difference tableau [8] shown below for the function $\phi[\xi] = \exp(\xi h_j)$:

$$\begin{array}{ccccccc}
\phi[\xi_1] & & & & & & \\
& \phi[\xi_1,\xi_2] & & & & & \\
\phi[\xi_2] & & \phi[\xi_1,\xi_2,\xi_3] & & & & \\
& \phi[\xi_2,\xi_3] & & \phi[\xi_1,\xi_2,\xi_3,\xi_4] & & & \\
\phi[\xi_3] & & \phi[\xi_2,\xi_3,\xi_4] & & & & \\
& \phi[\xi_3,\xi_4] & & & & & \\
\phi[\xi_4] & & & & & &
\end{array}$$

where $\xi_1 = ik_0\lambda_{1(j)}$, $\xi_2 = ik_0\lambda_{2(j)}$, $\xi_3 = ik_0\lambda_{3(j)}$ and $\xi_4 = ik_0\lambda_{4(j)}$. The r_i for (8) come from the upper diagonal of the tableau: $r_1(h_j) = \phi[\xi_1]$, $r_2(h_j) = \phi[\xi_1,\xi_2]$, $r_3(h_j) = \phi[\xi_1,\xi_2,\xi_3]$, and $r_4(h_j) = \phi[\xi_1,\xi_2,\xi_3,\xi_4]$. They require less arithmetic at each layer than the solution of the 4×4 system (10) for the coefficients c_i in the Cayley-Hamilton method.

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