An Application of Runge-Kutta Predictor-Corrector Methods To Two System of Hyperbolic Equations Arising in Optics[1]

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This work began a few years ago with a discussion I had at the University of Toronto with three physicists: C. M. de Sterke, B. D. Robert and J. E. Sipe. They were studying light propagation in nonlinear periodic media, which lead them to a model involving the *coupled-mode equations*

$$i\frac{\partial \mathcal{F}_+}{\partial t} + i\frac{\partial \mathcal{F}_+}{\partial z} = -\kappa\mathcal{F}_- - \Gamma|\mathcal{F}_+|^2\mathcal{F}_+ - 2\Gamma|\mathcal{F}_-|^2\mathcal{F}_+ \tag{1}$$

$$i\frac{\partial \mathcal{F}_-}{\partial t} - i\frac{\partial \mathcal{F}_-}{\partial z} = -\kappa\mathcal{F}_+ - \Gamma|\mathcal{F}_-|^2\mathcal{F}_- - 2\Gamma|\mathcal{F}_+|^2\mathcal{F}_- \tag{2}$$

on the domain $D = \{(t, z) : t \geq 0,\ z \in [0, b]\}$ with initial and boundary conditions

$$\mathcal{F}_\pm(0, z) = 0, \qquad \mathcal{F}_+(t, 0) = A(t), \qquad \mathcal{F}_-(t, b) = 0. \tag{3}$$

$\mathcal{F}_+$ and $\mathcal{F}_-$ denote the envelope functions of the forward and backward traveling modes, respectively, that determine the electrical field inside the system which has length b and is driven by radiation coming in at $z = 0$ with amplitude $A(t)$. Of particular interest are $\mathcal{F}_-(t, 0)$ and $\mathcal{F}_+(t, b)$, the amplitudes of the reflected and transmitted radiation, respectively. More details about the problem are given in [2] and the references therein.

Equations (1)–(3) constitute a well-posed hyperbolic initial-value problem with characteristics $t - z = c_1$ and $t + z = c_2$ for constants c_1 and c_2. Applying the transformations $z = \zeta - \tau$ and $t = \zeta + \tau$, we obtain the equations

$$i\frac{\partial \mathcal{F}_+}{\partial \zeta} = -\kappa\mathcal{F}_- - \Gamma|\mathcal{F}_+|^2\mathcal{F}_+ - 2\Gamma|\mathcal{F}_-|^2\mathcal{F}_+ \tag{4}$$

$$i\frac{\partial \mathcal{F}_-}{\partial \tau} = -\kappa\mathcal{F}_+ - \Gamma|\mathcal{F}_-|^2\mathcal{F}_- - 2\Gamma|\mathcal{F}_+|^2\mathcal{F}_- \tag{5}$$

which have a strong resemblance to ODEs, although they are not strictly speaking in this class. This observation lead de Sterke, Robert and Sipe to try to solve (1)–(3) numerically by the *method of characteristics*. They discretized the domain D as shown in Figure 1, where the stepsize is $h = b/L$ for some appropriately chosen integer L, $t_k = kh$ for $k = 0, 1, \ldots$, and $z_l = lh$ for $l = 0, 1, \ldots, L$. Their goal was to integrate (4) for $\mathcal{F}_+$ along the characteristic from (t_k, z_l) to (t_{k+1}, z_{l+1}) for $k = 0, 1, \ldots$ and $l = 0, 1, \ldots, L-1$ with initial conditions taken at $k = 0$ and $l = 0$, and similarly to integrate (5) for $\mathcal{F}_-$ along the characteristic from (t_k, z_l) to (t_{k+1}, z_{l-1}), for $k = 0, 1, \ldots$ and $l = 1, \ldots, L$ with initial conditions taken at $k = 0$ and $l = L$. (Ignore for now the vertical lines labeled N in Figure 1.)

If one uses a simple numerical scheme, such as Euler's method, to integrate (4)–(5), this approach leads to an easily implemented low-order method for solving (1)–(3). However, de Sterke, Robert and Sipe needed to solve the couple mode equations quite accurately over fairly long time intervals. Therefore, they wanted to use a higher-order scheme to solve (4)–(5).

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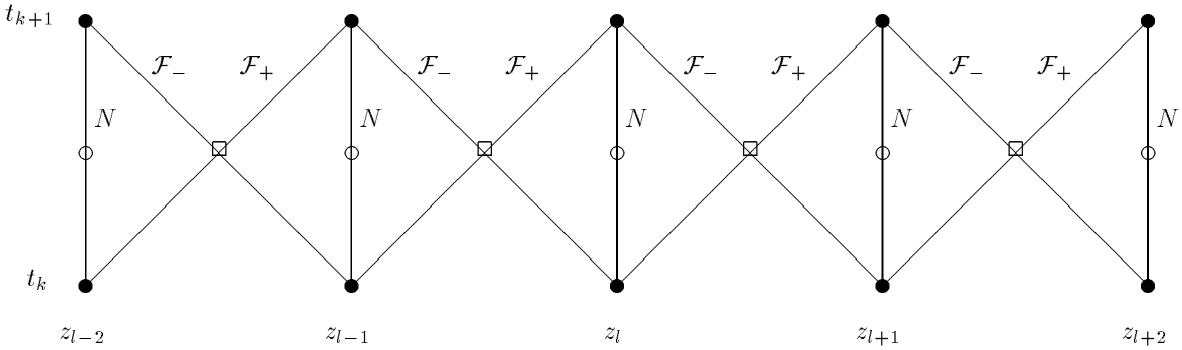

Figure 1: $\mathcal{F}_+$ is integrated along the characteristic from (t_k, z_l) to (t_{k+1}, z_{l+1}), $\mathcal{F}_-$ is integrated along the characteristic from (t_k, z_l) to (t_{k+1}, z_{l-1}), and N is integrated along the characteristic from (t_k, z_l) to (t_{k+1}, z_l).

Unfortunately, multistep methods appear inappropriate in this setting, since past values are not available for $\mathcal{F}_+$ at the boundaries $t = 0$ and $z = 0$ nor for $\mathcal{F}_-$ at the boundaries $t = 0$ and $z = b$. Moreover, the uniform characteristic-based grid shown in Figure 1 precludes starting the integration with a low-order multistep scheme requiring no past values and using a small stepsize and increasing the order, past values used and stepsize as the integration proceeds, as is often done in multistep codes for ODEs.

Therefore de Sterke, Robert and Sipe focused their attention on explicit Runge-Kutta (RK) methods. The difficulty for these schemes in this setting is that, when integrating (4) for $\mathcal{F}_+$, they need values for $\mathcal{F}_-$ at all points along the line joining (t_k, z_l) and (t_{k+1}, z_{l+1}) where the RK formula evaluates the right side of (4). We see from Figure 1 that such values are available only at the points $(t_k + mh/2, z_l + mh/2)$, where m is an integer. Moreover, for $m < 0$ or $m > 2$, the required values may lie outside the domain D, resulting in a problem like that described above for multistep formulas. A similar difficulty arises in the integration of (5) for $\mathcal{F}_-$. Consequently, they restricted their consideration to RK formulas with abscissae $c_i \in \{0, 1/2, 1\}$.

The classical fourth-order RK formula (RK4) has abscissae $c_i \in \{0, 1/2, 1\}$, and so seems like an appropriate scheme for this application. However, to apply RK4 to an ODE $y'(x) = f(x, y)$ on a step from x_n to x_{n+1}, you must evaluate $k_1 = f(x_n, y_n)$, $k_2 = f(x_n + h/2, y_n + hk_1/2)$, $k_3 = f(x_n + h/2, y_n + hk_2/2)$, and $k_4 = f(x_n + h, y_n + hk_3)$. The last of these, k_4, presents a problem in this setting. For example, when integrating (4) for $\mathcal{F}_+$ along the characteristic from (t_k, z_l) to (t_{k+1}, z_{l+1}), you need a "properly biased" value for $\mathcal{F}_-$ at (t_{k+1}, z_{l+1}) corresponding to $y_n + hk_3$. At the interior points of the grid, this value can be obtained from the integration of $\mathcal{F}_-$ along the characteristic from (t_k, z_{l+1}) to (t_{k+1}, z_l). But, at the boundary $z = b$, the latter line segment lies outside the domain. An alternative at $z = b$ is to use the boundary value $\mathcal{F}_-(t_{k+1}, z_L)$ in place of the value corresponding to $y_n + hk_3$. $\mathcal{F}_-(t_{k+1}, z_L)$, though, is not the properly biased value required by RK4, and for ODEs, at least, using such a value in place of the properly biased value $y_n + hk_3$ in k_4 results in a decrease in order for the formula. A similar difficulty arises in integrating $\mathcal{F}_-$ from (t_k, z_1) to (t_{k+1}, z_0). Since de Sterke, Robert and Sipe were not getting the accuracy they expected from RK4, we decided to try another method. It is not clear to me now, though, that their accuracy problems were due to their use of exact boundary values in place of the properly biased ones.

At that time, together with A. Kværnø, S. P. Nørsett and our students, I was investigating RK Predictor-Corrector (PC) methods [3, 4, 5, 6]. I suggested that de Sterke, Robert and Sipe try the RK–PC scheme

$$\left\{ \begin{array}{rcl} y^{(0)}_{n+1/2} &=& y_{n-1} + \dfrac{h}{8}\left[3f(x_{n-1}, y_{n-1}) + 9f(x_n, y_n)\right] \\ y^{(0)}_{n+1} &=& y_{n-1} + \dfrac{h}{3}\left[4f(x_{n-1}, y_{n-1}) - 8f(x_n - h/2, y_{n-1/2}) + 10f(x_n, y_n)\right] \end{array} \right\} \tag{6}$$

$$\left\{ \begin{array}{rcl} y^{(m)}_{n+1/2} &=& y_n + \dfrac{h}{24}\left[5f(x_n, y_n) + 8f(x_n + h/2, y^{(m-1)}_{n+1/2}) - f(x_{n+1}, y^{(m-1)}_{n+1})\right] \\ y^{(m)}_{n+1} &=& y_n + \dfrac{h}{6}\left[f(x_n, y_n) + 4f(x_n + h/2, y^{(m-1)}_{n+1/2}) - f(x_{n+1}, y^{(m-1)}_{n+1})\right] \end{array} \right\} \tag{7}$$

where $m = 1, 2, \ldots, M$ in (7) and we take $y_{n+1/2} = y_{n+1/2}^{(M)}$ and $y_{n+1} = y_{n+1}^{(M)}$ for a suitably chosen M. If you remove the superscripts in (7), then the resulting formula is a fourth-order three-stage RK scheme based on quadratic collocation at the points $\{x_n,\ x_n + h/2,\ x_{n+1}\}$. The predictor (6) uses the collocation polynomial from the previous step to predict the starting values $y_{n+1/2}^{(0)}$ and $y_{n+1}^{(0)}$ for the corrector (7), as explained in more detail in [1, 2].

My original interest in RK–PC schemes like (6)–(7) stems from the observation that all the function evaluations needed in each iteration of (6) or (7) can be performed simultaneously, making these schemes attractive for parallel computation. However, the scheme (6)–(7) also seems well suited for the solution of (4)–(5). In particular, because (7) is based on a collocation scheme, when integrating (4) for $\mathcal{F}_+$ along the characteristic from (t_k, z_{L-1}) to (t_{k+1}, z_L), it is quite appropriate to use $\mathcal{F}_-(t_{k+1}, z_L)$ in place of the $\mathcal{F}_-$ value corresponding to $y_{n+1}^{(m-1)}$. Moreover, because the predictor (6) is accurate, only one or two iterations of (7) are needed at most points. The exceptions are at the start of the iteration ($t = 0$) for both $\mathcal{F}_+$ and $\mathcal{F}_-$, at the boundary $z = 0$ for $\mathcal{F}_+$, and at the boundary $z = b$ for $\mathcal{F}_-$. At these points, (6) is not applicable because the past values corresponding to y_{n-1} and $y_{n-1/2}$ are not available. However, we can overcome this difficulty by iterating (7) a few extra times at these exceptional points, as described in more detail in [2]. This does not add significantly to the computational work required to solve (4)–(5).

Broderick and de Sterke later extended the model (1)–(3) to include the effect of free carriers on the refractive index of the medium. The resulting differential equations for $\mathcal{F}_+$ and $\mathcal{F}_-$ are similar to (1)–(2) except that the two right most term are replaced by $-\delta(N)\mathcal{F}_+$ in (1) and by $-\delta(N)\mathcal{F}_-$ in (2), where $\delta(N) = \frac{2\pi K_e}{\lambda} N$, K_e and λ are constants, $N(t, z)$ is a function that satisfies

$$\frac{\partial N}{\partial t} = \frac{\alpha}{h\nu}\left[\frac{2n}{Z}\left(|\mathcal{F}_+|^2 + |\mathcal{F}_-|^2\right)\right] - \frac{N}{T_c} \tag{8}$$

α, $h\nu$, n, Z, T_c are physical constants given in [1], not to be confused with any values of the same name used earlier. The associated initial condition is $N(0, z) = 0$ for $z \in [0, b]$. A change-of-variables similar to the one used to transform (1)–(2) to (4)–(5) leads to a set of three differential equations consisting of (8) and modified versions of (4) and (5). These are solved along the characteristics shown in Figure 1. A complicating factor here is that, when integrating (8) for N, values corresponding to $y_{n+1/2}$ for $\mathcal{F}_+$ and $\mathcal{F}_-$ are not available at the points marked $\circ$ in Figure 1. Similarly, when integrating (4) for $\mathcal{F}_+$ or (5) for $\mathcal{F}_-$, values corresponding to $y_{n+1/2}$ for N are not available at the points marked $\square$ in Figure 1. In our extended scheme, these missing values are replaced by approximations computed from four neighbouring values along the line $t = t_k + h/2$, as explained in more detail in [1]. The resulting scheme seems to retain the fourth-order convergence property of the RK–PC method (6)–(7).

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