The Numerical Solution of Coupled Integro-Differential Equations

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1. Introduction. The purpose of this paper is to report on a method for the numerical solution of simultaneous integro-differential equations of the form

$$\int_0^\infty \sum_{n=0}^{n_{\max}} ({}_1k_n(x, g)g^{(n)}(r))\, dy = \sum_{n=0}^{n_{\max}} {}_1P_n(x)f^{(n)}(x)$$

$$\int_0^\infty \sum_{n=0}^{n_{\max}} ({}_2k_n(r, \theta)f^{(n)}(x))\, d\theta = \sum_{n=0}^{n_{\max}} {}_2P_n(r)g^{(n)}(r)$$

where the asymptotic forms of $f(x)$ and $g(r)$ are known; and where ${}_1k_n$ and ${}_2k_n$ are the kernels. The method, which is reasonably simple to program for a computer, has been tested on a problem arising in nuclear physics and yielded reasonable results.

2. Motivation. A great deal of effort has gone into evolving satisfactory numerical methods of solutions of differential equations. Much less has been done in the field of integral equations; Fox and Goodwin [1] have given methods for solutions of equations of the form

$$\int_a^b k(x, y)f(y)\, dy = p(x) + f(x) \tag{2.1}$$

where $p(x)$ and $k(x, y)$ are known functions. Their method is to write the left-hand side of equation (2.1) in its finite difference form

$$\int_a^{b=a+mh} k(x, y)f(y)\, dy = \sum_{n=0}^{m} A_n\, k(x, nh)f(nh) + \pi_x \tag{2.2}$$

where A_n are the coefficients and π_x the truncation error of the particular quadrature chosen. The substitution of equation (2.2) into equation (2.1) for $x = a, a + h, a + 2h, \cdots, a + mh$, gives $m + 1$ simultaneous equations in π_x and the $m + 1$ unknowns $f(a), f(a + h), \cdots, f(a + mh)$. The truncation errors π_x may be made negligible by suitable choice of step-length or treated by the iterative scheme given by Fox and Goodwin; the equations may then be solved by any of the standard methods.

In the same paper they note that this method extends itself immediately to integro-differential equations of the following form

$$\int_a^b k(x, y)f(y)\, dy = P_0(x) + f(x) + \sum_{n=1}^{m} p_n(x)f^{(n)}(x) \tag{2.3}$$

where $f^{(n)}(x)$ is the nth derivative of $f(x)$, and $k(x, y)$ and $p_n(x)$ are known functions. The only additional substitution needed is the appropriate finite difference approximation for the derivatives. The treatment of the end points depends upon the boundary conditions, but in general causes no trouble.

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There arise in nuclear physics equations of the following form:

$$\int_0^\infty \sum_{n=0}^{n_{\max}} ({}_1k_n(x, g) g^{(n)}(r))\, dy = \sum_{n=0}^{n_{\max}} {}_1P_n(x) f^{(n)}(x) \tag{2.4}$$

$$\int_0^\infty \sum_{n=0}^{n_{\max}} ({}_2k_n(r, \theta) f^{(n)}(x))\, d\theta = \sum_{n=0}^{n_{\max}} {}_2P_n(r) g^{(n)}(x) \tag{2.5}$$

where x, y and r, θ are related coordinates

$$\begin{aligned} x &= \alpha(r, \theta) \\ y &= p(r, \theta). \end{aligned} \tag{2.6}$$

The problem is to compute a table of values of $f(x)$ and $g(r)$ for $x = r = a$, $x = r = a + h, \cdots, x = r = a + mh$ (these values of x and r will be referred to as the mesh points).

Equations (2.4) and (2.5) differ from equation (2.3) in the following significant respects:

a) The appearance of the derivatives of the unknown function in the integrand

b) The infinite interval of integration; that is, the equations are singular in the sense of Fox and Goodwin

c) The appearance of two naturally occurring coordinate systems; a finite difference mesh at even intervals in one coordinate system does not in general represent even intervals in the other. This reflects the fact that (2.4) and (2.5) are two-dimensional equations, although only of a restricted type.

3. Method. The method of Fox and Goodwin can nonetheless be used, but with appropriate modifications, to take care of the above difficulties:

a) The derivative under the integral sign may be replaced by an appropriate finite difference approximation; for example, the second difference might be used for the second derivative.

b) The infinite integrals can be made finite if there is a point beyond which the contributions of the integrand are negligible. However, in general, this will involve values of x and r outside the range in which the solution is desired.

c) Any two of the four coordinates determine the other two by relation (2.6). For example, in equation (2.4) r takes on the values $a, a + h, \cdots, a + mh$; but for a given r it is necessary to integrate over y. Each combination of r and y gives by equation (2.6) a value of x which may or may not be a mesh point. Two cases naturally follow:

a) $a < x < a + mh$ but $x \neq a + ih$ inside the mesh $i = 0, 1, 2, \cdots, m$

b) $x < a$ or $a + mh < x$ outside the mesh.

The first difficulty may be taken care of by interpolation. If, for example, linear interpolation is chosen and x lies between the mesh points x_i and x_{i+1}

$$f(x) = f(x_i)q + f(x_{i+1})p$$

$$p = 1 - q \qquad p = \frac{x - x_i}{x_{i+1} - x_1} \qquad x_i < x < x_{i+1}$$

Similarly, after substitution of the second difference,

$$f''(x) = pf(x_{i+2}) + (3q - 2)f(x_{i+1}) + (3p - 2)f(x_i) + qf(x_{i-1}) \quad x_i < x < x_{i+1}.$$

Alternatively, if x lies beyond the end values of the mesh, it is possible to employ the (assumed known) asymptotic forms of $f(x)$ and $g(r)$. Here the assumption is made that the last two mesh points $x = r = a + (m - 1)h$ and $x = r = a + mh$ are in the range of validity of the asymptotic forms. Suppose, for example, the asymptotic form of $f(x)$ is known to be

$$f(x) \to A\phi_1(x) + B\phi_2(x) \qquad x \to \infty \tag{3.1}$$

where ϕ_1 and ϕ_2 are known functions; and A and B are unknown constants to be determined *a posteriori* from the solution of the problem. Thus by our assumption

$$\begin{aligned} f(a + (m - 1)h) &= A\phi_1(a + (m - 1)h) + B\phi_2(a + (m - 1)h) \\ f(a + mh) &= A\phi_1(a + mh) + B\phi_2(a + mh) \end{aligned}$$

A and B can thus be solved for in terms of the two unknown end values $f(a + (m - 1)h)$, $f(a + mh)$; and these expressions can in turn be substituted back into equation (3.1) giving

$$\begin{aligned} f(x) \to {} & \frac{1}{\begin{vmatrix} \phi_1(a - (m - 1)h) & \phi_2(a + (m - 1)h) \\ \phi_1(a + mh) & \phi_2(a + mh) \end{vmatrix}} \\ & \cdot \left(\begin{vmatrix} f(a + (m - 1)h) & \phi_2(a + (m - 1)h) \\ f(a + mh) & \phi_2(a + mh) \end{vmatrix} \phi_1(x) + \right. \\ & \left. \begin{vmatrix} \phi_1(a + (m - 1)h) & f(a + (m - 1)h) \\ \phi_1(a + mh) & f(a + mh) \end{vmatrix} \phi_2(x) \right) \\ = {} & f(a + (m - 1)h) \frac{1}{\begin{vmatrix} \phi_1(a + (m - 1)h) & \phi_2(a + (m - 1)h) \\ \phi_1(a + mh) & \phi_2(a + mh) \end{vmatrix}} (\phi_2(a + mh)\phi_1(x) \\ & - \phi_1(a + mh)\phi_2(x)) + f(a + mh) \frac{1}{\begin{vmatrix} \phi_1(a + (m - 1)h) & \phi_2(a + (m - 1)h) \\ \phi_1(a + mh) & \phi_2(a + mh) \end{vmatrix}} \\ & \cdot (\phi_1(a + (m - 1)h)\phi_2(x) - \phi_2(a + (m - 1)h)\phi_1(x)). \end{aligned}$$

Thus if x is not a mesh point, it is possible by interpolation and the use of the asymptotic form to express $f(x)$ in terms of the value at mesh points. In the same fashion the difficulties are overcome in equation (2.5) when r takes on the values $r = a, r = a + h, \cdots, r = a + mh$.

The appropriate mesh size, interval of integration and cut-off point for the infinite integral depend upon the problem.

4. Example. In the discussion of neutron-deuteron scattering by the resonating group method including inelastic channels [3], the following equations arise:

$$\frac{3}{2}\cdot\frac{d^2f(x)}{dx^2}+\frac{2m}{h^2}(E-E_d)f(x)+\frac{2m}{h^2}\frac{V_0 r_0^2 f(x)}{x}\int_0^\infty G_0(x,y)\,dy$$

$$+x\int_0^\infty\left(r^{-5/2}\frac{d^2g(n)}{dr^2}-\frac{15}{4}r^{-9/2}g(r)\right)\phi(y)y\,dy+\frac{2m}{h^2}x \tag{4.1}$$

$$\cdot\int_0^\infty G_1(x,y)g(r)\,dy=0$$

$$\frac{16}{\sqrt{3\pi}}r^{1/2}\int_0^{\pi/2}\left(\frac{3}{2}\frac{d^2f(x)}{dx^2}+G_2(r,\alpha)f(x)\right)\phi(y)\sin\alpha\cos\alpha\,d\alpha+\frac{d^2g(r)}{dr^2}$$

$$\cdot\frac{-15}{4r^2}g(r)+\frac{2mE}{h^2}g(r)+\frac{2m}{h^2}g(r)\int_0^{\pi/2}G_3(r,\alpha)\sin^2\alpha\cos^2\alpha\,d\alpha=0 \tag{4.2}$$

$$x=\sqrt{\tfrac{3}{2}}r\cos\alpha\qquad y=\sqrt{2}r\sin\alpha$$

$$G_0=\frac{\phi^2(y)}{y}\exp\left[-\frac{1}{r_0^2}\left(x^2+\frac{y^2}{4}\right)\right]\left[\exp\frac{xy}{r_0^2}-\exp\left(-\frac{xy}{r_0^2}\right)\right]$$

$$G_1=\frac{\phi(y)}{r^{5/2}}y\left[E+V_0\exp\left(-\frac{y_0^2}{r_0^2}\right)+\frac{V_0 r_0^2}{xy}\right.$$

$$\left.\cdot\exp\left[-\frac{1}{r_0^2}\left(x^2+\frac{y^2}{4}\right)\right]\left[\exp\left(\frac{xy}{r_0^2}\right)-\exp\left(\frac{-xy}{r_0^2}\right)\right]\right]$$

$$G_2=\frac{2m}{h^2}\left[E-E_d+\frac{V_0 r_0^2}{xy}\exp\left[-\frac{1}{r_0^2}\left(x^2+\frac{y^2}{4}\right)\right]\right. \tag{4.3}$$

$$\left.\cdot\left[\exp\left(\frac{xy}{r_0^2}\right)-\exp\left(-\frac{xy}{r_0^2}\right)\right]\right]$$

$$G_3=\frac{16V_0}{\pi}\left[\exp\left(-\frac{y^2}{r_0^2}\right)+\frac{r_0^2}{xy}\exp\left[-\frac{1}{r_0^2}\left(x^2+\frac{y^2}{4}\right)\right]\right]$$

$$\cdot\left[\exp\left(\frac{xy}{r_0^2}\right)-\exp\left(\frac{-xy}{r_0^2}\right)\right].$$

The physical interpretation of the various quantities is as follows: $\phi(y)$ is the bound-state deuteron function satisfying the equation

$$\left[\frac{d^2}{dy^2}+\frac{2m}{h^2}\left(V_0\exp\left(-\frac{y^2}{r_0^2}\right)+E_d\right)\right]\phi(y)=0.$$

For large y it falls off exponentially:

$$\phi(y)\to A\exp(-k_d y)\qquad h^2k_d=-mE_d$$

The function $\phi(y)$ and the eigenvalue V_0 were calculated numerically by a separate program.

E_d is the (negative) deuteron energy; m the mass of a nucleon. The potential between two nucleons is the Gaussian form $-V_0\exp\left(-\frac{r^2}{r_0^2}\right)$.

The unknowns $f(x)$ and $g(r)$ represent respectively the elastic and inelastic scattering wave functions.

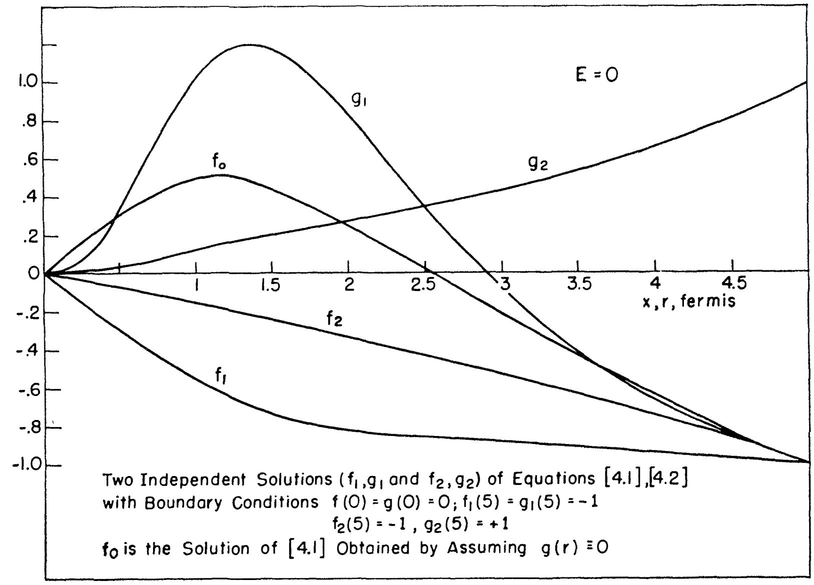

FIG. 1.

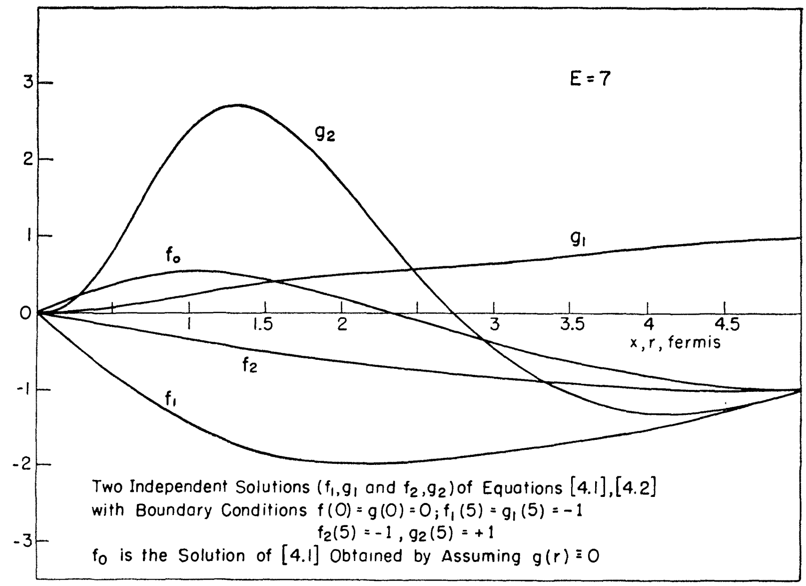

FIG. 2.

The equations are of the form of equations (2.4) and (2.5), and have been solved by the methods described here. The asymptotic forms of $f(x)$ and $g(r)$ are

$$\begin{aligned} f(x) &= A \sin (k_n x) + B \cos (k_n x) \qquad 2h^2 k_n = 3m(E - E_d) \quad x \to \infty \\ g(r) &= C r^{1/2} J_2(kr) + D r^{1/2} N_2(kr) \qquad h^2 k^2 = 2mE \quad r \to \infty \end{aligned} \tag{4.4}$$

where $J_n(z)$ and $N_n(z)$ are the Bessel functions of the first and second kind of order n as defined in Jahnke and Emde [2].

The application of the above techniques for solving the equations is straightforward. The integrals of infinite range converge rather slowly, so that the back interpolation (equation (3.2)) has to be applied over a wide range of r; however, this can be avoided in this example by noting that for r such that equation (4.4) is valid

$$\left(r^{-5/2}\frac{d^2}{dr^2} - \frac{15}{4r^{9/2}} + \frac{2m}{h^2}G_1\right)g(r) = 0$$

since this reduces to the Bessel equation satisfied by $g(r)$. The second and third integrals in equation (4.1) can then be cut off at this point, which is long before the individual terms are negligible. Moreover, the first integral converges very rapidly and is negligible even before this cutoff point is reached. The equations have been solved in particular cases both with and without taking note of this point; the results were comparable but the computing time was reduced from fifteen to three minutes. Difference corrections were neglected; the mesh size was varied until stability was reached with the accuracy required ($\sim$3%). Figures 1 and 2 give a plot of the results of runs for $E = 0$, $E = 7$; the constants used were (lengths in units of 10^{-13} cm; energies in Mev)

$$r_0 = 1.332 \quad V_0 = 86.674 \quad E_d = -2.226 \quad \frac{2m}{h^2} = .0481933$$

$$h(y) = .2 \quad h(x) = .25 = h(r) \quad E = 5.$$

The asymptotic form was used for r, $x \geqq 4.75$. Other runs were made for $E = 0.5, 1, 3, 5$; for $E = 0$, the asymptotic form for $g(r)$ is modified. Also plotted in Figures 1 and 2 are the results obtained by solving equation (4.1) for $f(x)$ setting $g(r) = 0$ (physically, neglecting the effect of the inelastic channel upon the elastic channel). For further detail of the numerical results see [3]. Higher values of E were not used because the end point of the mesh used ($r = 5$) is close to a zero of $g(r)$ for E of the order of 10.

The problem was coded in SAP for the IBM 704 at M.I.T. Coding was straightforward; the most laborious task was debugging—a single suitable hand check took several days to complete. The program was approximately 2,000 instructions long. Running time for the coefficients from (4.1) was from 2.5 to 7 minutes depending upon mesh size; 2 minutes for the coefficients from equation (4.2), and one minute for the matrix solution.

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