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# Numerical Integration of A Nonlinear, Singular Integro-Partial Differential Equation

K. KRISHNA PRASAD* AND R. G. HERING

*University of Illinois at Urbana–Champaign, Urbana, Illinois 61801*

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A method for numerical integration of a nonlinear, singular integro-partial differential equation is presented. The method consists in evaluating the singular integral by a least-squares approximation technique. A predictor–corrector formula is employed to integrat the ordinary differential equations obtained after the spatial discretization of the partial integrodifferential operator. Results of the procedure developed are compared with those obtained with the Newton–Gregory formula for evaluating the integral. Numerical results are presented to illustrate the effectiveness and accuracy of the algorithm. The influence of parameters in the equation on the behavior of the algorithm is discussed.

## INTRODUCTION

Nonlinear integral equations frequently arise in physical problems and, except for isolated instances, must be solved numerically. Noble [1] reviewed numerical solution methods for nonlinear integral equations. Although an exhaustive literature is available on numerical solution of ordinary and partial differential equations [2], this situation does not exist for nonlinear integrodifferential operators, especially when partial derivatives are present. The present study describes a numerical integration technique developed for a nonlinear integro-partial differential equation which may be extended to equations of the same general character. The equation considered is

$$\frac{\partial f}{\partial t} = \frac{1}{2}\left[E_2(y) + f_1^4 E_2(Y - y) - 2f^4(y, t) + \int_0^Y f^4(y', t)\, E_1(|\, y - y' \,|)\, dy'\right] \quad (1)$$

with the initial condition

$$f(y, 0) = f_1 . \quad (2)$$

The functions $E_n(x)$ are exponential integral functions of order $n$ [3] and are

* Present address: Department of Mechanical Engineering, Indian Institute of Science, Bangalore-12, India.

available only in tabulated form. The parameters $f_1$ and $Y$ are specified constants. The development of Eq. (1) is given elsewhere [4]. For the present purpose it is sufficient to state that Eq. (1) governs the local temperature during transient radiative heat transfer in a plane layer of absorbing material bounded by black walls. The layer is initially at unit temperature when the lower wall ($y = 0$) is suddenly changed to temperature $f_1$ while the upper wall ($y = Y$) is maintained at the initial temperature. In this application $f(y, t)$ denotes dimensionless local temperature, $y$ and $t$ are dimensionless space and time variables, and $Y$ is the optical thickness of the layer.

Numerical solution to Eq. (1) is complicated by the fact that the kernel of the integral $E_1(| y - y' |)$ is singular at the origin although the integral exists and is finite. In principle the initial value problem represented by Eq. (1) with the initial condition of Eq. (2) can be integrated to steady state ($t \to \infty$) where transient effects vanish identically in a manner analogous to parabolic differential equations. In the latter case, however, theoretical results are available [5] for selecting increments in the independent variables which assure stability and convergence of the numerical integration process. No such results are apparently available for integration of equations of the type considered here. It is reasonable to expect, however, that a stable difference method for integrating the differential equation is suitable provided an accurate quadrature rule is chosen to evaluate the integral. Thus, integration of Eq. (1) is considered in two parts. First, techniques for the evaluation of the singular integral are described. An approximation for the time derivative is then discussed. Finally, numerical results are presented illustrating the application and accuracy of the method developed.

## Numerical Evaluation of a Singular Integral

Noble [1] has considered the evaluation of singular integrals treating them as Cauchy principal-value integrals using methods of interpolation and approximation.

The first method divides the range of integration into three subintervals, with one of them containing the singularity and the other two free from it. The integration over the latter two can be performed by a standard interpolative scheme. The former can be evaluated by expanding $f^4(y', t)$ in a Taylor's series around $y$ and the resulting integrals are evaluated in closed form in terms of $E_n$.

This method is not attractive for integrating Eq. (1). However, limited calculations were performed for $Y = 1$ using the Newton–Gregory formula. The method was found unsatisfactory in regard to the amount of computer time required to achieve acceptable accuracy, even with as many as 200 spatial approximation points. It may be mentioned that the Newton–Gregory formula uses available

values of the function at the approximation points, thus avoiding interpolation among the points. Some numerical results in this connection are cited later.

Approximation methods represent the function $f^4(y', t)$ by a finite expansion in terms of elementary functions. Since moments of $E_n$ functions are simple to evaluate, it is convenient to use polynomials orthogonal over the set of approximation points. Thus, the function $f^4(y, t)$ is approximated as

$$f^4(y, t) = \sum_{j=0}^{k} B_j(t)\, p_j(y), \tag{3}$$

where $p_j(y)$ is the polynomial of order $j$ in the space variable $y$. The time-dependent coefficients $B_j(t)$ can be calculated by a least-squares procedure. The smoothing properties of this procedure tend to reduce the influence of small errors introduced at any step of the integration process on subsequent results. For $Y$ around 1 the number of approximation points required is about one third of the points needed for the quadrature method discussed earlier. This leads to a considerable reduction in computation time required to integrate Eq. (1).

The orthogonal polynomials were constructed by adapting an algorithm given by Anderson [6] to the discrete situation. Double precision arithmetic was employed to minimise the adverse round-off properties of the algorithm. To promote speed and accuracy of computation, the interval of integration in Eq. (1) was normalized to $(-0.5, 0.5)$ and the approximation points were chosen symmetric with respect to zero, with the result that all odd-power coefficients for even-degree polynomials and all even-power coefficients for odd-degree polynomials vanish. By this procedure it was possible to generate polynomials orthogonal to within $10^{-15}$ for orders up to 25 and number of approximation points up to 200, when care was taken to adjust the value of the inner product $(p_j, p_j)$ to unity. The least-squares approximation was generated by a method suggested by Forsythe [7]. Though the assumptions of the above work are not truly valid in the present case, it was found that its use produced better approximations than a test for small error norm. For all approximations generated, polynomials of degree higher than 15 were found unnecessary since the error vector variance, $\sigma^2$, varied slowly for higher degree polynomials and was usually between $10^{-5}$ and $10^{-8}$. Since the approximation was used for quadrature purposes, this order of accuracy was considered adequate.

Spatial discretization of Eq. (1) and subsequent use of the polynomial approximation yields

$$\frac{df^{(n)}}{dt} = \frac{1}{2}\left[E_2(y_n) + f_1^4 E_2(Y - y_n) + \sum_{j=0}^{k} B_j(t)\, \psi_{jn} - 2\{f^{(n)}(t)\}^4\right], \tag{4}$$

$$f^{(n)}(0) = f_1 \qquad (n = 0, 1, 2, \ldots, N), \tag{5}$$

where the $f^{(n)}$ are the discrete approximations to $f$ over the set of space points $y_n$ ($n = 0, 1, 2, \ldots, N$) and

$$\begin{aligned} \psi_{jn} &= \int_0^Y p_j(y')\, E_1(|\, y_n - y' \,|)\, dy' \\ &= \sum_{i=0}^{j} A_{ij} \int_0^Y y'^i E_1(|\, y_n - y' \,|)\, dy'. \end{aligned} \tag{6}$$

The $p_j$ are the polynomials discussed earlier and the $A_{ij}$ are the coefficients of these polynomials. Note that for a selected distribution of approximation points, degree of approximation [i.e., $k$ in Eq. (3)], and $Y$, the $\psi_{jn}$ may be calculated independently of the integration procedure for Eq. (4), which is in contrast to the repetitive calculation required for the interpolative method.

## Numerical Integration Method

The system given in Eq. (4) is a set of ordinary simultaneous differential equations with initial conditions prescribed by Eq. (5). They were integrated using a fourth-order predictor-corrector formula due to Hamming [8].

The convergence rate of the corrector formula determines the computation time and is governed by the nature of the function on the right side of Eq. (4). In the present application the behavior of this function is strongly determined by the kernel $E_1(|\, y - y' \,|)$, which is singular at $y = y'$ and decreases exponentially with increasing $y - y'$. The mode of convergence is strongly dependent on a 'characteristic width' ($\lambda$) of the kernel function. For large $\lambda$ (corresponding to small $Y$) a strong global coupling exists among all $f^{(n)}$ values while for small $\lambda$ (large $Y$) there is principally only a local coupling among $f^{(n)}$ values. For small $\lambda$ the ordinary iterative scheme tends to become ill-conditioned. Complete discussion of this problem and alternative iterative schemes has been given by Anderson [9]. For the present problem the ill-conditioning attains significant proportions for $Y$ larger than three or four. This behavior thus places an additional restriction on the choice of the value for the time increment and, in general, it is necessary to exercise caution when step lengths are changed during integration.

The time increment was chosen so that corrector iterations were generally limited to two and decreased on the basis of truncation error which registered an automatic increase in situations where corrector convergence was poor. The step length was increased principally on the basis of the physical requirement that after some time the local temperature variation with time decreases, enabling larger time steps to be employed, and not on the basis of truncation error which is the customary criterion in the case of ordinary differential equations.

The starting values for the predictor–corrector formula were obtained by a fourth-order Runge–Kutta procedure. Integration was terminated by appealing to the physical situation at steady state (as $t \to \infty$). At steady state the function $f(y, t)$, nondimensionalized as

$$\bar{f} = \frac{f^4 - f_1^4}{1 - f_1^4},$$

satisfies

$$\bar{f}\left(\frac{y}{Y}\right) = 1 - \bar{f}\left(1 - \frac{y}{Y}\right). \tag{7}$$

The validity of Eq. (7) may be demonstrated by substituting it into Eq. (1) after the time derivative is set to zero. It follows that $\bar{f}(0.5) = 0.5$. The integration procedure was terminated when $\bar{f}(0.5)$ was within 0.01 % of this value. The quality of the integration procedure can be gauged by another physical fact. At steady state the radiative flux which is the integral of the right side of Eq. (1) over the space coordinate must be uniform.

## Results and Discussion

Because of the complex nature of Eq. (1) and the approximations involved, mathematical analysis to establish the convergence, stability, and error bounds for the numerical scheme was not attempted. Instead, independent error estimates for the integration of the system expressed by Eq. (4) with Eq. (5) and the least-squares approximation were obtained [7, 8]. A summary of typical error estimates obtained during integration is shown in Table I.

The ad hoc procedure of halving the time interval was adopted to investigate convergence of the procedure. Stability of the method was established by study of the extent to which the results satisfied the physical requirement that radiative flux be uniform in [0, $Y$] at steady state ($t \to \infty$). Typical steady state flux results are presented in Tables II and III for the algorithm developed as well as some of those obtained using the Newton–Gregory formula. For identical parameter values, the least-squares procedure yields uniformity of flux to four significant figures. Results obtained using the Newton–Gregory formula are satisfactory to only two significant figures with errors for the boundary surface flux exceeding 5 %. Physically the boundary fluxes are important quantities obtained from the calculation. It may also be noted that the number of approximation points used for the least-squares method is 21, while 101 were required for the Newton–Gregory formula. This situation permits a small time increment to be used at early time in the least-squares method. Such small step lengths are prohibitively time con-

TABLE I

Typical Error Estimates During Integration ($Y = 0.1, f_1 = 0.5$)

| $t$ | Step length | $y/Y$ | Degree of polynomial | Variance ($\times 10^8$) | Number of corrector iterations | Truncation error ($\times 10^8$) |
|---|---|---|---|---|---|---|
| 0.060 | 0.010 | | 6 | 0.56 | 2 | |
| | | 0.00 | | | | −6.5 |
| | | 0.25 | | | | −1.2 |
| | | 0.50 | | | | −0.44 |
| | | 0.75 | | | | +0.33 |
| | | 1.00 | | | | +5.7 |
| 1.130 | 0.020 | | 15 | 8.0 | 2 | |
| | | 0.00 | | | | −0.44 |
| | | 0.25 | | | | −0.44 |
| | | 0.50 | | | | −0.44 |
| | | 0.75 | | | | −0.22 |
| | | 1.00 | | | | −0.33 |
| 3.670 | 0.040 | | 15 | 52.0 | 2 | |
| | | 0.00 | | | | −0.55 |
| | | 0.25 | | | | −0.33 |
| | | 0.50 | | | | −0.44 |
| | | 0.75 | | | | −0.33 |
| | | 1.00 | | | | −0.44 |
| 7.71 | 0.080 | | 15 | 140.0 | 2 | |
| | | 0.00 | | | | −0.55 |
| | | 0.25 | | | | −0.44 |
| | | 0.50 | | | | −0.39 |
| | | 0.75 | | | | −0.39 |
| | | 1.00 | | | | −0.33 |
| 14.35 | 0.160 | | 15 | 380.0 | 2 | |
| | | 0.00 | | | | −0.55 |
| | | 0.25 | | | | −0.44 |
| | | 0.50 | | | | −0.44 |
| | | 0.75 | | | | −0.33 |
| | | 1.00 | | | | −0.39 |

Note : 1. Number of approximation points = 81.
2. Highest degree of polynomial employed = 15.
3. Step length was increased every hundred steps.

suming with the Newton–Gregory formula. The latter calculation procedure was found to be at least 10 to 20 times slower than that required in the least-squares method. In both integration methods step length was increased during the integration.

TABLE II

Flux Distribution Obtained by Using Least-Squares Approximations ($Y = 1.0, f_1 = 2/3$)

| | $t$ | | | |
|---|---|---|---|---|
| $y/Y$ | 3.030 | 4.070 | 6.510 | 9.070 |
| 0.0 | 0.117270 | 0.113263 | 0.111210 | 0.111032 |
| 0.1 | 0.116586 | 0.113038 | 0.111217 | 0.111042 |
| 0.2 | 0.115685 | 0.112733 | 0.111179 | 0.111041 |
| 0.3 | 0.114612 | 0.112355 | 0.111158 | 0.111037 |
| 0.4 | 0.113313 | 0.111914 | 0.111115 | 0.111035 |
| 0.5 | 0.111866 | 0.111409 | 0.111064 | 0.111031 |
| 0.6 | 0.110336 | 0.110856 | 0.111023 | 0.111028 |
| 0.7 | 0.108720 | 0.110258 | 0.110974 | 0.111025 |
| 0.8 | 0.107050 | 0.109637 | 0.110908 | 0.111020 |
| 0.9 | 0.105460 | 0.109013 | 0.110861 | 0.111014 |
| 1.0 | 0.104000 | 0.108426 | 0.110780 | 0.110998 |

Note: 1. Number of approximation points = 21.
2. Maximum degree of polynomial employed = 15.
3. Time increment = 0.01.

TABLE III

Flux Distribution Obtained by Using the Newton–Gregory Formula
($Y = 1.0, f_1 = 2/3, h = 0.01$)

| | $t$ | | | |
|---|---|---|---|---|
| $y/Y$ | 3.000 | 4.100 | 6.500 | 9.300 |
| 0.0 | 0.116626 | 0.112194 | 0.110135 | 0.10994 |
| 0.1 | 0.113937 | 0.109525 | 0.108073 | 0.107897 |
| 0.2 | 0.114022 | 0.110336 | 0.109117 | 0.108967 |
| 0.3 | 0.113879 | 0.111348 | 0.110591 | 0.109995 |
| 0.4 | 0.113475 | 0.111883 | 0.111955 | 0.110979 |
| 0.5 | 0.112856 | 0.112311 | 0.112803 | 0.111919 |
| 0.6 | 0.112058 | 0.112640 | 0.113604 | 0.112816 |
| 0.7 | 0.111127 | 0.112880 | 0.113987 | 0.113669 |
| 0.8 | 0.110119 | 0.113049 | 0.114359 | 0.114080 |
| 0.9 | 0.109108 | 0.113172 | 0.115072 | 0.114870 |
| 1.0 | 0.108210 | 0.113304 | 0.115764 | 0.115998 |

Note: 1. Differences up to fourth order were retained in the quadrature formula.
2. In the Taylor expansion for $f^4(y', t)$ for evaluation of the integral around the singular point, derivatives up to third order were retained.
3. Time increment = 0.05.

The degree of instability in the least-squares procedure can be established readily by forming difference tables for $\bar{f}$. Table IV presents typical differences up to third order at large times for $Y = 1.0$, $f_1 = 0.5$, and three values of $y/Y$ (0, 0.5, and 1.0). The tabular results indicate that the instability is of the order of few digits in the fifth significant figure and thus assures results accurate to four significant figures.

TABLE IV

Large Time Difference Tables ($Y = 1.0, f_1 = 0.5$)

| | $y/Y = 0.0$ | | | | $y/Y = 0.5$ | | | | $y/Y = 1.0$ | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $t$ | $\bar{f}$ | $\Delta$ | $\Delta^2$ | $\Delta^3$ | $\bar{f}$ | $\Delta$ | $\Delta^2$ | $\Delta^3$ | $\bar{f}$ | $\Delta$ | $\Delta^2$ | $\Delta^3$ |
| 3.87 | 0.73672 | | | | 0.44616 | | | | 0.19449 | | | |
| | | 543 | | | | 1287 | | | | 992 | | |
| 4.19 | 0.74215 | | 123 | | 0.45903 | | 299 | | 0.20441 | | 184 | |
| | | 420 | | 27 | | 988 | | 67 | | 808 | | 24 |
| 4.51 | 0.74635 | | 96 | | 0.46891 | | 232 | | 0.21249 | | 160 | |
| | | 324 | | 23 | | 756 | | 52 | | 648 | | 24 |
| 4.83 | 0.74959 | | 73 | | 0.47647 | | 180 | | 0.21897 | | 136 | |
| | | 251 | | 15 | | 576 | | 42 | | 512 | | 23 |
| 5.15 | 0.75210 | | 58 | | 0.48223 | | 138 | | 0.22409 | | 113 | |
| | | 193 | | 14 | | 438 | | 33 | | 399 | | 23 |
| 5.47 | 0.75403 | | 44 | | 0.48661 | | 105 | | 0.22808 | | 90 | |
| | | 149 | | 11 | | 333 | | 25 | | 309 | | 18 |
| 5.79 | 0.75552 | | 33 | | 0.48994 | | 80 | | 0.23117 | | 72 | |
| | | 116 | | 6 | | 253 | | 18 | | 237 | | 15 |
| 6.11 | 0.75668 | | 27 | | 0.49247 | | 62 | | 0.23354 | | 57 | |
| | | 89 | | 8 | | 191 | | 16 | | 180 | | 14 |
| 6.43 | 0.75757 | | 19 | | 0.49438 | | 46 | | 0.23534 | | 43 | |
| | | 70 | | 3 | | 145 | | 10 | | 137 | | 9 |
| 6.75 | 0.75827 | | 16 | | 0.49583 | | 36 | | 0.23671 | | 34 | |
| | | 54 | | 5 | | 109 | | 10 | | 103 | | 8 |
| 7.07 | 0.75881 | | 11 | | 0.49692 | | 26 | | 0.23774 | | 26 | |
| | | 43 | | 3 | | 83 | | 6 | | 77 | | 6 |
| 7.39 | 0.75924 | | 8 | | 0.49775 | | 20 | | 0.23851 | | 20 | |
| | | 35 | | | | 63 | | | | 57 | | |
| 7.71 | 0.75959 | | | | 0.49838 | | | | 0.23908 | | | |

Available steady-state results [10] for $\bar{f}$ were compared with the present results providing an additional check on the calculations. It should be pointed out that under steady conditions Eq. (1) simplifies to a linear integral equation in $f^4(y, t)$. The reported results are shown in Table V for three values of $Y$. Errors are generally of the order of 1 % and less.

It is appropriate at this stage to comment on the influence of $f_1$ and $Y$ on the integration. In general there is a need for increasing the number of approximation points as $Y$ is increased or $f_1$ is reduced ($0 < Y < \infty$, $0 < f_1 < 1$). With the number of approximation points 80 or less, it is possible to carry out the integration for $Y < 2$ for all $f_1$. As a rule, it is possible to manage with even fewer approximation points for these situations provided a smaller time step is chosen. However, choice of too small a time step leads to an undesirable buildup of round-off errors, particularly for $Y > 1$, since a large number of steps is required to attain steady state. The optimum step length and the number of approximation points were chosen empirically.

TABLE V

Comparison of Steady-State Temperature Distributions

| $Y$ | 0.1 | | 1.0 | | 10.0 | |
|---|---|---|---|---|---|---|
| $y/Y$ | Heaslet–Warming [12] | Present study | Heaslet–Warming [12] | Present study | Heaslet–Warming [12] | Present study |
| 0.0 | 0.571 | 0.571 | 0.756 | 0.760 | 0.956 | 0.949 |
| 0.1 | 0.556 | 0.554 | 0.698 | 0.692 | 0.854 | 0.851 |
| 0.2 | 0.541 | 0.539 | 0.646 | 0.642 | 0.765 | 0.763 |
| 0.3 | 0.525 | 0.526 | 0.590 | 0.594 | 0.678 | 0.675 |
| 0.4 | 0.513 | 0.512 | 0.551 | 0.545 | 0.590 | 0.587 |
| 0.5 | 0.500 | 0.499 | 0.500 | 0.499 | 0.500 | 0.499 |
| 0.6 | 0.487 | 0.486 | 0.449 | 0.452 | 0.410 | 0.412 |
| 0.7 | 0.475 | 0.473 | 0.410 | 0.405 | 0.322 | 0.324 |
| 0.8 | 0.459 | 0.460 | 0.354 | 0.355 | 0.235 | 0.236 |
| 0.9 | 0.444 | 0.446 | 0.302 | 0.305 | 0.146 | 0.148 |
| 1.0 | 0.429 | 0.428 | 0.244 | 0.240 | 0.044 | 0.050 |

The procedure developed is not very satisfactory for large $Y$, say around 10. In such situations, the kernel function tends to reproduce the function at points distant from the boundaries and the forcing function $\{E_2(y) + f_1^4 E_2(Y - y)\}$ strongly influences only points close to the boundary. The least-squares approximation produces erratic results in such cases at "early times" and the errors introduced tend to grow with time. This presents a formidable obstacle for the integration. However, the integration can be carried out satisfactorily by using the following procedure. It is assumed that the least-squares fit produces adequate accuracy for $f$ in the region $0 < y/Y < 0.6$. Near this point the value of the right side of Eq. (1) tends to be negative, which is physically absurd. For larger values

of $y/Y$, the function $f$ was maintained at its initial value. As integration proceeds, this "cut-off" point gradually moved toward the boundary, $y/Y = 1$. Once the "cut-off" point reached the boundary integration progressed smoothly. Due to the ill-conditioning of the iterative process of the corrector, the size of the time step is severely restricted. This sometimes gives a large buildup of round-off errors.

## Conclusion

A numerical method of solution for a nonlinear, integropartial differential equation with a singular kernel has been presented. The technique uses least-squares approximation for the function within the integral operator to reduce the equation to a system of ordinary differential equations. Hamming's predictor–corrector formula is employed to solve the differential equation system. Although considerable information of an experimental nature has been obtained on the effectiveness of the solution method in handling problems of the class considered here, further study of the technique should be initiated to fully explore the potential of the technique. In particular more information concerning the relation between the error in the least-squares approximation and the behavior of the predictor–corrector formula is needed.

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