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The Use of Symbolic Computation in Radiative, Energy,
 and Neutron Transport Calculations

by

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Summary:

This investigation uses symbolic computation in developing analytical methods and general computational strategies for solving both linear and nonlinear, regular and singular, integral and integro-differential equations which appear in radiative and combined mode energy transport.

This technical report summarizes the research conducted during the first nine months of the present investigation. The use of Chebyshev polynomials augmented with symbolic computation has clearly been demonstrated in problems involving radiative (or neutron) transport, and mixed-mode energy transport. Theoretical issues related to convergence, errors, and accuracy have also been pursued. Three manuscripts have resulted from the funded research. These manuscripts have been submitted to archival journals (one has been accepted in the *Quarterly of Applied Mathematics*).

At the present time, an investigation involving a conductive and radiative medium is underway. The mathematical formulation leads to a system of nonlinear, weakly-singular integral equations involving the unknown temperature and various Legendre moments of the radiative intensity in a participating medium. Some preliminary results are presented illustrating the direction of the proposed research.

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Appendix A:

Paper entitled: "Several Symbolic Augmented Cheyshev Expansions for Solving the Equation of Radiative Transfer" by J.I. Frankel, Ph.D. *Journal of Computational Physics*, (in review)

Appendix B:

Paper entitled: "A Galerkin Solution to a Regularized Cauchy Singular Integro-Differential Equation" by J.I. Frankel, Ph.D., *Quarterly of Applied Mathematics* (accepted for publication).

Appendix C:

Paper entitled: "Generalization of the Method of Peters to Cauchy Singular Integro-Differential Equations", by J.I. Frankel, Ph.D., *Proceedings of the Royal Society of London, Series A* (in review).

Acknowledgement: The author wishes to thank Mr. T. LaClair for preparing the finite element results presented in Tables 4 and 5 of this report.

I. INTRODUCTION

In radiative, neutron, and energy transport, complicated mathematical models are normally developed. Typically, nonlinear integral and integro-differential equations, and nonlinear differential equations are produced through the modeling process. The degree of complexity usually depends on the level of sophistication associated with the model. Once a satisfactory mathematical model has been produced, the next step involves the numerical simulation of the mathematical expressions used in relating the physical phenomena to the mathematical description.

In light of the complicated mathematical structure associated with radiative, neutron, and energy transport, new solution methods which exploit symbolic computation appear to be the natural extension of classical doctrine. Indeed, classical expansion methods as well as numerical computation can be augmented with the aid of symbolic computation. Alternative mathematical formulations may produce new forms which are clearly receptive to symbolic computation.

The work summarized here promotes alternative mathematical formulations based on integral equations for producing a mathematical environment which permits the use of expansion methods augmented by symbolic computation. This produces excellent numerical results to a class of difficult energy related problems. Potential impact could affect problems involving combustion, nuclear fission and fusion, solar energy and other energy topics.

II. PROGRESS AND PRESENT ACTIVITIES

The accurate solution of complicated nonlinear, weakly-singular, coupled Fredholm integral equations has potential impact to numerous energy related problems. In particular, we wish to demonstrate (and later generalized) the use of symbolic computation in promoting the development of accurate approximate analytic and numeric solutions.

During the course of the present investigation, several objectives have been set forth including:

- a) To demonstrate the usefulness and robustness of symbolic computation used in conjunction with creative analysis,
- b) To systematically study representative problems related to energy transport and to develop new techniques and formulations which promote the use of symbolic computation for developing analytic and numeric solutions, and

- c) To illustrate a logical sequence of representative problems which can be used as stepping stones to advanced and practical problems related to MHD, nuclear fission and fusion, combustion, and solar energy.

Several additional objectives have been considered during the first nine months of the present study including:

- a) To develop expertise with both Mathematica™ and Maple on a NeXT TurboStation and to understand the limitations of such software,
- b) To develop a high level of expertise with Chebyshev polynomials, and
- c) To develop a sequence of problems which permit clear understanding leading to the development of general software programs for solving a large class of transport problems.

As an example of the context of the research program, consider the classical problem of mixed conductive and radiative transport in a participating, isotropically scattering, plane-parallel medium. The following dimensionless equations (see Siegel and Howell [1, p. 830]) govern the first law of thermodynamics (energy) and the integral form of the equation of radiative transport:

Energy Equation:

$$\frac{d^2\theta}{dn^2}(\eta) = \frac{4\alpha^2(1-\omega)}{\lambda\omega}[\theta^+(\eta) - G(\eta)], \quad \eta \in (-1,1), \quad (1a)$$

subject to

$$\theta(-1) = 1, \quad (1b)$$

$$\theta(1) = \theta_2, \quad (1c)$$

Integral Form of the Equation of Radiative Transport:

$$G(\eta) = (1-\omega)\theta^+(\eta) + \frac{\omega}{2}[E_2(\alpha(1+\eta)) + \theta_2^+ E_2(\alpha(1-\eta))] + \frac{\alpha\omega}{2} \int_{\eta-1}^1 G(\xi) E_1(\alpha|\eta-\xi|) d\xi, \quad \eta \in [-1,1]. \quad (2)$$

where $\theta(\eta)$ is the dimensionless temperature, $G(\eta)$ is the zeroth moment of the radiative intensity (see [1] for further details).

This system is representative of a larger set of practical problems involving combined radiative and conductive energy transport. One can generalize this problem further to include convection and highly anisotropic scattering. This will be the subject of the second year. Demonstration of several new concepts have been the subject of the first year of research. A cohesive and systematic approach leading to the accurate solution of equations similar to that displayed in Eqs. (1-2) has been the primary focus of the first year of research.

Accomplishments to Date (15 August 1992 - 1 May 1993):

Three manuscripts have been prepared and submitted to archival journals. Copies of these manuscripts are presented in Appendices A-C. The manuscript entitled: "A Galerkin Solution to a Regularized Cauchy Singular Integro-Differential Equation" by J.I. Frankel has been accepted for publication in the Quarterly of Applied Mathematics. The accepted version is displayed in Appendix B. This paper presents a new formulation of and subsequent solution using Chebyhev polynomials to the Cess and Tiwari problem described in the original DOE proposal (see pages 8 -10). Algebraic manipulations were augmented by symbolic computation. A generalized and expanded study was presented in the paper entitled "Generalization of the Method of Peters to Cauchy Singular Integro-Differential Equations" by J.I. Frankel (enclosed as Appendix C)

The manuscript entitled "Several Symbolic Augmented Chebyshev Expansions for Solving the Equation of Radiative Transfer" by J.I. Frankel (submitted to the Journal of Computational Physics) illustrated several important uses of symbolic computation (algebra, integration, and graphics). In addition, it is apparently the first work to use Chebyshev polynomials as the basis functions for solving the integral form of the transport equation. In as such, much effort was exerted into understanding theoretical issues involving the rate of convergence, rigorous error bounds, and accuracy monitoring. Three expansion techniques were systematically studied. The three methods considered were: 1) point collocation, 2) Ritz-Galerkin, and 3) weighted-Galerkin. Appendix A should be consulted for detailed information.

In a nutshell, the integral form of the transport equation was considered in an isotropically scattering plane-parallel medium, namely

$$G(\eta) = f^\alpha(\eta) + \frac{\lambda}{2} \int_{\eta-1}^1 E_1(\alpha|\xi - \eta|)G(\xi)d\xi, \quad \eta \in [-1,1]. \quad (3)$$

Here $G(\eta)$ represent the zeroth moment of intensity as defined by

$$G(\eta) = 2\pi \int_{\mu=-1}^1 I(\eta,\mu)d\mu, \quad \eta \in [-1,1], \quad (4)$$

where $I(\eta,\mu)$ is the local radiative intensity. The kernel shown in Eq. (3) is the first exponential integral function [1] which contains a logarithmic singularity as the argument tends to zero. Thus, Eq. (3) is described as a weakly-singular (integrable) Fredholm integral of the second kind for the unknown function $G(\eta)$. The known forcing function is denoted by $f^\alpha(\eta)$. The function $G(\eta)$ has practical importance since one can directly arrive at the radiative heat flux, divergence of the radiative heat flux and two important surface properties (reflectivity and transmissivity) once $G(\eta)$ is resolved.

The present solution approach relies on expansion techniques. Of particular interest (and merit) is the use of Chebyshev polynomials as the basis functions. Explicitly, we express the unknown function $G(\eta)$ as

$$G(\eta) = \sum_{m=0}^{\infty} a_m^* T_m(\eta), \quad \eta \in [-1,1], \quad (5)$$

where $T_m(\eta)$ is the m^{th} Chebyshev polynomial of the first kind [2,3]. These polynomials have several exploitable features and follow numerous well-known relations. As with any expansion technique, the main goal lies in determining the unknown expansion coefficients $\{a_m^*\}$, $m = 0, \dots$ in an accurate and rapid manner.

In general, we must seek an approximate solution to $G(\eta)$ by truncating the infinite series shown in Eq. (5) at a certain order N , namely

$$G_N(\eta) = \sum_{m=0}^N a_m^N T_m(\eta), \quad \eta \in [-1,1], \quad (6)$$

where a_m^N is an approximation to a_m^* for each fixed m . Equation (3) now can be expressed as

$$R_N(\eta) = G_N(\eta) - f^\alpha(\eta) - \frac{\lambda}{2} \int_{\eta-1}^1 E_1(\alpha|\xi - \eta|)G_N(\xi)d\xi, \quad \eta \in [-1,1], \quad \lambda > 0, \quad \alpha > 0. \quad (7)$$

Here, $R_N(\eta)$ is the local residual functions. The local error can be expressed as

$$\epsilon_N(\eta) = G(\eta) - G_N(\eta). \quad (8)$$

From our definition of the local error function $\epsilon_N(\eta)$, and using Eqs. (3) and (7), we can derive an exact integral equation for the local error in terms of the residual function

$R_N(\eta)$, namely

$$R_N(\eta) = -\epsilon_N(\eta) + \frac{\lambda}{2} \int_{\eta-1}^1 E_1(\alpha|\eta - \xi|) \epsilon_N(\xi) d\xi, \quad \xi \in [-1, 1]. \quad (9a)$$

(Note: In general, the residual function $R_N(\eta)$ will have an oscillatory nature.) From this, we can obtain the rigorous error bound

$$\frac{\|R_N\|_p}{1 + \frac{\lambda}{2}\|K\|_p} \leq \|\epsilon_N\|_p \leq \frac{\|R_N\|_p}{1 - \frac{\lambda}{2}\|K\|_p}, \quad (9b)$$

(when $1 - \frac{\lambda}{2}\|K\|_p > 0$). Here, the p^{th} functional norm of $R_N(\eta)$ is denoted as $\|R_N\|_p$, and the p^{th} operator norm of K is expressed as $\|K\|_p$. Note that K denotes an integral operator such as defined by

$$Kg = \int_{\eta-1}^1 K(\eta, \xi) g(\xi) d\xi, \quad (10)$$

where $K(\eta, \xi)$ is the kernel and g represents some unknown function.

Through exploitation of several features offered by Mathematica™ (and some of Maple), an approximate solution for $G_N(\eta)$ can be obtained using a minimal amount of computer code using the three expansion methods previously discussed. Figure 1 displays the solution for $G_N(\eta)$ and the residual functions $R_N(\eta)$ for the three expansion methods used in the study when $\omega = 0.8$, $L = 2$ and $N = 7$. Here ω represents the single-scatter albedo and L represents the optical thickness.

Table 1 presents some representative results (see Appendix A for further results) illustrating the effectiveness of the collocation approach for determining the surface properties R and T (i.e., reflectivity and transmissivity, respectively) for various albedos and optical thicknesses. Table 2 presents the effect of coupling among the expansion coefficients as a function of the number of terms retained in the series representation for the unknown function $G_N(\eta)$. The upper and lower L_∞ -error bounds are also presented in this table. It is interesting to note that most researchers have "demonstrated" accuracy in their numerical schemes by mere comparison with the surface properties R and T . It is clear that 4 significant figures of accuracy is possible to obtain with regard to the surface properties without having 4 significant figures of accuracy in $G_N(\eta)$. This is expected owing to the definitions of R and T (see Appendix A).

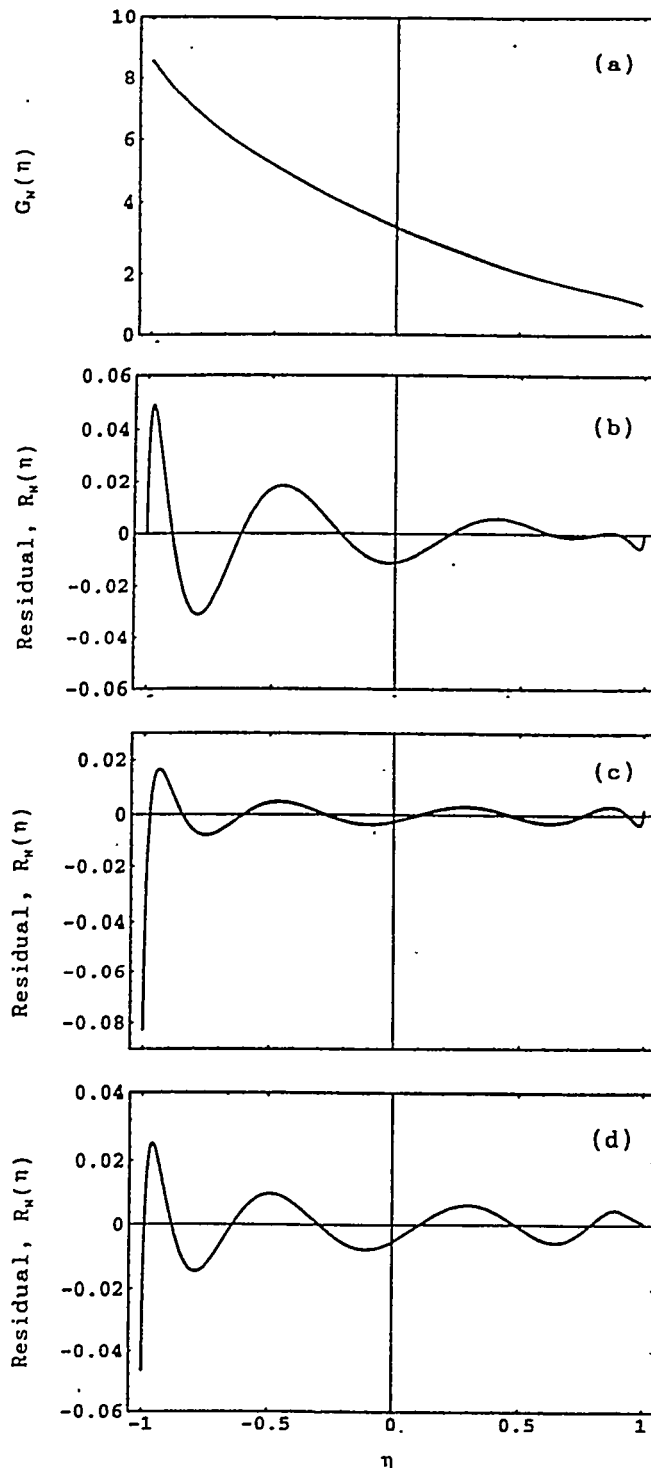


Figure 1. The approximate solution, $G_N(\eta)$ and residual plots, $R_N(\eta)$ for the methods of b) collocation, c) Ritz-Galerkin, and d) weighted-Galerkin ($N=7$, $\omega=0.8$, $L=2$).

| ω | Surface Property | $L = 0.5 (N=7)$ | | $L = 1 (N=7)$ | | $L = 2 (N=9)$ | | $L = 5 (N=11)$ | |
|----------|------------------|-----------------|--------|---------------|--------|---------------|--------|----------------|--------|
| | | Present | Exact | Present | Exact | Present | Exact | Present | Exact |
| 0.995 | R | 0.2932 | 0.2932 | 0.4412 | 0.4412 | 0.5988 | 0.5888 | 0.7636 | 0.7636 |
| | T | 0.7018 | 0.7018 | 0.5488 | 0.5488 | 0.3815 | 0.3815 | 0.1892 | 0.1892 |
| 0.9 | R | 0.2475 | 0.2475 | 0.3527 | 0.3527 | 0.4372 | 0.4376 | 0.4764 | 0.4763 |
| | T | 0.6599 | 0.6599 | 0.4747 | 0.4747 | 0.2656 | 0.2656 | 0.0634 | 0.0534 |
| 0.8 | R | 0.2056 | 0.2056 | 0.2802 | 0.2806 | 0.3280 | 0.3280 | 0.3417 | 0.3417 |
| | T | 0.6220 | 0.6220 | 0.4162 | 0.4162 | 0.1973 | 0.1973 | 0.0229 | 0.0229 |
| 0.7 | R | 0.1690 | 0.1690 | 0.2221 | 0.2221 | 0.2506 | 0.2506 | 0.2566 | 0.2565 |
| | T | 0.5891 | 0.5891 | 0.3712 | 0.3712 | 0.1551 | 0.1551 | 0.0124 | 0.0124 |
| 0.6 | R | 0.1365 | 0.1365 | 0.1743 | 0.1743 | 0.1919 | 0.1919 | 0.1948 | 0.1947 |
| | T | 0.5603 | 0.5603 | 0.3356 | 0.3355 | 0.1269 | 0.1269 | 0.0077 | 0.0077 |
| 0.5 | R | 0.1077 | 0.1077 | 0.1342 | 0.1342 | 0.1451 | 0.1451 | 0.1466 | 0.1456 |
| | T | 0.5350 | 0.5350 | 0.3067 | 0.3067 | 0.1071 | 0.1071 | 0.0053 | 0.0053 |
| 0.3 | R | 0.0584 | 0.0584 | 0.0701 | 0.0701 | 0.0741 | 0.0741 | 0.0745 | 0.0745 |
| | T | 0.4924 | 0.4925 | 0.2631 | 0.2631 | 0.0814 | 0.0814 | 0.0030 | 0.0030 |
| 0.1 | R | 0.0178 | 0.0178 | 0.0208 | 0.0207 | 0.0216 | 0.0216 | 0.0217 | 0.0217 |
| | T | 0.4580 | 0.4578 | 0.2319 | 0.2317 | 0.0659 | 0.0658 | 0.0021 | 0.0020 |

Table 1. Comparison of the present collocation results for R and T to the exact results for various optical thicknesses, L and albedos, ω .

| a_k^N | $N = 3$ | $N = 5$ | $N = 7$ | $N = 9$ | $N = 11$ | $N = 13$ |
|---------------|-----------|------------|------------|-------------|-------------|-------------|
| a_0^N | 4.00079 | 3.97947 | 3.97582 | 3.97469 | 3.97424 | 3.97402 |
| a_1^N | -3.58873 | -3.50197 | -3.49091 | -3.48776 | -3.48652 | -3.48593 |
| a_2^N | 0.823741 | 0.732223 | 0.722387 | 0.719784 | 0.718793 | 0.718333 |
| a_3^N | -0.242179 | -0.257857 | -0.239203 | -0.235060 | -0.233589 | -0.232929 |
| a_4^N | | 0.0976552 | 0.0774224 | 0.073513 | 0.0722306 | 0.0716811 |
| a_5^N | | -0.0490953 | -0.0575897 | -0.0505265 | -0.0484691 | -0.0476382 |
| a_6^N | | | 0.0318984 | 0.0245541 | 0.0226228 | 0.0218904 |
| a_7^N | | | -0.0185276 | -0.0233762 | -0.0200245 | -0.0188587 |
| a_8^N | | | | 0.0145546 | 0.0112132 | 0.0101349 |
| a_9^N | | | | -0.00890106 | -0.0118907 | -0.0100779 |
| a_{10}^N | | | | | 0.0078602 | 0.00611486 |
| a_{11}^N | | | | | -0.00493661 | -0.00690141 |
| a_{12}^N | | | | | | 0.00472646 |
| a_{13}^N | | | | | | -0.00301481 |
| R | 0.332869 | 0.328332 | 0.328015 | 0.327968 | 0.327957 | 0.327954 |
| T | 0.195848 | 0.197152 | 0.197253 | 0.197266 | 0.197268 | 0.197269 |
| $\ e_N\ _m^U$ | 0.668451 | 0.283302 | 0.153469 | 0.0954606 | 0.0648849 | 0.0468881 |
| $\ e_N\ _m^L$ | 0.126754 | 0.0537207 | 0.0291013 | 0.0181016 | 0.0123037 | 0.0088911 |

Table 2. Convergence of the collocation expansion coefficients when $\omega = 0.8$ and $L = 2$.

Table 3 displays some results comparing the numerically obtained L_∞ -error bound as determined by numerical means from Eq. (9a) to the upper and lower bounds for the case when $\omega = 0.8$, and $L = 2$. Clearly, the actual error tends toward the lower-error bound rapidly for this particular case.

Appendix A presents illustrative results for the three expansion methods. Detailed error analysis and the establishment of the rate of convergence for the collocation method has been developed with aid of a projection method [4-7]. The details are presented in Appendix A.

From this study, it is clear that the integral form of the Boltzmann transport equation which appears in both radiative and neutron transport theories can be exploited by symbolic computation. In particular, an expansion method using Chebyshev polynomials as the basis function is worthy of additional pursuit. Indeed the extension to highly anisotropic scattering phase functions now appears at hand.

Present Investigation (1 April 1993 - 14 August 1993)

A candidate solution approach based on the integral form of the radiative equation of transfer has been successfully tested. Before proceeding to investigate the coupled system displayed in Eqs. (1)-(2), it is appropriate to explore some new avenues involving the formulation of the energy equation. Equation (1) is a nonlinear differential equation for the unknown temperature $\Theta(\eta)$ which is coupled with the unknown function $G(\eta)$. Some special remarks should now be made with regard to the approach to be taken here.

Unlike traditional doctrine, which emphasizes direct numerical simulation of the governing system or the use of multiple expansion forms for $\Theta(\eta)$ and $\Theta^4(\eta)$, we plan to take a consistent approach based on an expansion method.

To illustrate the approach without introducing undue complication in the presentation, consider the differential equation

$$\frac{d^2\Theta}{d\eta^2}(\eta) - \beta^2\Theta^4(\eta) = 0, \quad \eta \in (-1,1), \tag{11a}$$

subject to

$$\Theta(-1) = 1, \tag{11b}$$

$$\Theta(1) = \Theta_2. \tag{11c}$$

Note that this is rather reminiscent of Eq. (1) but without the unknown function $G(\eta)$. For example, this equation has physical

| N | $\ e_N\ _{\infty}^L$ | $\ e_N\ _{\infty}^2$ | $\ e_N\ _{\infty}^U$ |
|-----|----------------------|----------------------|----------------------|
| 1 | 0.5373 | 2.17 | 2.834 |
| 2 | 0.2513 | 0.71 | 1.325 |
| 3 | 0.1268 | 0.28 | 0.6685 |
| 4 | 0.08079 | 0.16 | 0.4261 |
| 5 | 0.05372 | 0.0987 | 0.2833 |
| 6 | 0.0391 | 0.069 | 0.2063 |
| 7 | 0.02913 | 0.051 | 0.1535 |
| 8 | 0.02280 | 0.039 | 0.1202 |
| 9 | 0.01810 | | 0.09546 |
| 10 | 0.01486 | | 0.07835 |
| 11 | 0.01230 | | 0.06489 |
| 12 | 0.01043 | | 0.05498 |
| 13 | 0.008891 | | 0.04689 |

Table 3. Error bounds (L_{∞} -norm) for the collocation method when $\omega = 0.8$ and $L = 2$.

meaning with regard to steady, one-dimensional, conduction and surface radiation in a spline geometry.

One can easily recast Eq. (11a-c) into the equivalent integral equation with the aid of Green's functions [8]. Doing so yields

$$\Theta(\eta) = f(\eta) - \beta^2 \int_{\eta_0}^1 G(\eta, \eta_0) \Theta^4(\eta_0) d\eta_0, \quad \eta \in [-1, 1], \quad (12a)$$

where

$$f(\eta) = G_{\eta_0}(\eta, -1) - \Theta_2 G_{\eta_0}(\eta, 1), \quad (12b)$$

and where $G(\eta, \eta_0)$ is the two-point Green's function

$$G(\eta, \eta_0) = \begin{cases} \frac{(1 - \eta)(1 + \eta_0)}{2}, & -1 \leq \eta_0 \leq \eta, \\ \frac{(1 - \eta_0)(1 + \eta)}{2}, & \eta \leq \eta_0 \leq 1. \end{cases} \quad (12c)$$

Equation (12a) is representative of a Hammerstein [5,9,10] integral equation. At first glance, one is tempted to immediately expand $\Theta(\eta)$ as

$$\Theta(\eta) = \sum_{n=0}^{\infty} b_n^* T_n(\eta), \quad \eta \in [-1, 1], \quad (13)$$

and substitute it into Eq. (12a). However, this operation should cause some concern owing to necessity of taking the fourth power of the series representation. Since the system is nonlinear, one expects to find the unknown expansion coefficients by some iterative means. Thus, it appears that direct substitution of Eq. (13) into Eq. (12a) could require the evaluation of the integral term at each iterate.

Recently, Kumar and Sloan [11] presented a simple way around this dilemma by defining a new function, namely

$$\Psi(\eta) = \Theta^4(\eta), \quad (14)$$

and upon substituting this into Eq. (12a), we arrive at

$$\Theta(\eta) = f(\eta) - \beta^2 \int_{\eta_0}^1 G(\eta, \eta_0) \Psi(\eta_0) d\eta_0, \quad \eta \in [-1, 1]. \quad (15)$$

Next, we substitute Eq. (15) into Eq. (14) to arrive at

$$\Psi(\eta) = [f(\eta) - \beta^2 \int_{\eta_0}^1 G(\eta, \eta_0) \Psi(\eta_0) d\eta_0]^4, \quad \eta \in [-1, 1]. \quad (16)$$

Thus, if we can determine $\Psi(\eta)$ by some means we can back out $\Theta(\eta)$ through Eq. (15). Let the unknown function, $\Psi(\eta)$ be represented by the expansion

$$\Psi(\eta) = \sum_{n=0}^{\infty} c_n^N T_n(\eta), \quad \eta \in [-1,1]. \quad (17)$$

Approximating $\Psi(\eta)$ by $\Psi_N(\eta)$ produces

$$\Psi_N(\eta) = \sum_{n=0}^N c_n^N T_n(\eta), \quad \eta \in [-1,1], \quad (18)$$

and upon substituting Eq. (18) into Eq. (16), we arrive at

$$R_N(\eta) = - \sum_{n=0}^N c_n^N T_n(\eta) + [f(\eta) - \beta^2 \sum_{n=0}^N (a_n^N C_n(\eta))]^4, \quad (19a)$$

where

$$C_m(\eta) = \int_{\eta_c=-1}^{\eta_c=1} G(\eta, \eta_c) T_m(\eta_c) d\eta_c, \quad m = 0,1,\dots,N. \quad (19b)$$

Clearly, this type manipulation allows for the direct analytic integration of $C_m(\eta)$, $m=0,1,\dots,N$ independent of the unknown expansion coefficients (in fact, this is a single time evaluation for each m). To determine the unknown expansion coefficients by the collocation method, we require

$$\langle R_N(\eta), \Omega_k(\eta) \rangle_{w_k} = 0, \quad k = 0,1,\dots,N, \quad (20)$$

where $w_k = \delta(\eta - \eta_k)$, $\Omega_k(\eta) = 1$. Thus, we arrive $N+1$ simultaneous nonlinear algebraic equations for the expansion coefficients $\{a_n^N\}$, $m = 0,1,\dots,N$, namely

$$0 = - \sum_{n=0}^N c_n^N T_n(\eta_k) + [f(\eta_k) - \beta^2 \sum_{n=0}^N (a_n^N C_n(\eta_k))]^4, \quad k = 0,1,\dots,N. \quad (21)$$

Here we defined the collocation points as

$$\eta_k = \cos\left[\frac{\pi k}{N}\right], \quad k = 0,1,\dots,N. \quad (22)$$

Unfortunately, both Mathematica and Maple have difficulties in solving large systems ($N>3$) of nonlinear algebraic equations in a reliable fashion. Thus, a simple under-relaxed, Gauss-Seidel method has been successfully implemented using the Mathematica language. Presently, we are developing a Newton-Raphson [12] method which is well-suited for this class of problem.

Tables 4 and 5 present some preliminary results for $\Theta(\eta)$ when $\Theta_2 = 0.2$ and $\beta = 0.1, 1$, respectively. As shown in Table 4, it appears that the collocation solution converges quite rapidly (as expected for a weakly nonlinear system). As the strength of the nonlinearity increases, rapid convergence still takes place. The finite element solution (using linear elements) clearly indicates that as β increase the number of elements increases substantially in order to obtain 4 places of accuracy.

| n | Finite Element Solution | | Integral Equation | |
|------|-------------------------|--------|-------------------|--------|
| | N = 20 | N = 50 | N = 3 | N = 5 |
| -1 | 1 | 1 | 1 | 1 |
| -0.8 | 0.9194 | 0.9194 | 0.9194 | 0.9194 |
| -0.6 | 0.8391 | 0.8391 | 0.8391 | 0.8391 |
| -0.4 | 0.7589 | 0.7589 | 0.7590 | 0.7589 |
| -0.2 | 0.6790 | 0.6790 | 0.6790 | 0.6790 |
| 0 | 0.5991 | 0.5991 | 0.5991 | 0.5991 |
| 0.2 | 0.5192 | 0.5192 | 0.5192 | 0.5192 |
| 0.4 | 0.4394 | 0.4394 | 0.4394 | 0.4394 |
| 0.6 | 0.3596 | 0.3596 | 0.3596 | 0.3596 |
| 0.8 | 0.2798 | 0.2798 | 0.2798 | 0.2798 |
| 1 | 0.2 | 0.2 | 0.2 | 0.2 |

Table 4 Results for $\Theta(\eta)$ comparing FEM solution to the proposed Chebyshev-collocation solution when $\beta = 0.1$, $\Theta_2 = 0.2$ using the Green's function indicated in Eq. (12c).

| n | Finite Element Solution | | | Integral Equation | |
|------|-------------------------|--------|---------|-------------------|--------|
| | N = 20 | N = 50 | N = 100 | N = 3 | N = 5 |
| -1 | 1 | 1 | 1 | 1 | 1 |
| -0.8 | 0.8742 | 0.8743 | 0.8743 | 0.8743 | 0.8744 |
| -0.6 | 0.7724 | 0.7725 | 0.7726 | 0.7746 | 0.7728 |
| -0.4 | 0.6852 | 0.6854 | 0.6854 | 0.6905 | 0.6855 |
| -0.2 | 0.6070 | 0.6072 | 0.6072 | 0.6149 | 0.6070 |
| 0 | 0.5344 | 0.5346 | 0.5346 | 0.5433 | 0.5343 |
| 0.2 | 0.4651 | 0.4652 | 0.4653 | 0.4732 | 0.4650 |
| 0.4 | 0.3978 | 0.3979 | 0.3979 | 0.4038 | 0.3978 |
| 0.6 | 0.3314 | 0.3315 | 0.3315 | 0.3350 | 0.3316 |
| 0.8 | 0.2656 | 0.2656 | 0.2657 | 0.2671 | 0.2657 |
| 1 | 0.2 | 0.2 | 0.2 | 0.2 | 0.2 |

Table 5 Results for $\Theta(\eta)$ comparing FEM solution to the proposed Chebyshev-collocation solution when $\beta = 1$, $\Theta_2 = 0.2$ using the Green's function indicated in Eq. (12c).

Figure 2 presents $\Theta(\eta)$ for $\beta = 0.1$ and 1 when $\Theta_2 = 0.2$. As $\beta \rightarrow 0$, a linear distribution results. Figure 3 presents the residual function for both cases corresponding to Figure 2 when $N = 5$. The oscillatory nature of the residual is clearly seen along with the true locations of the chosen $N + 1$ collocation points.

At the present time, error analysis is underway. At first glance, the original formulation shown in Eq. (12a) appears to be more amenable to error analysis than the formulation displayed in Eq. (16). This is presently under scrutiny.

The choice of Green's function is rather arbitrary (i.e., not unique) since it depends on the operator being inverted. Clearly, the choice shown in Eq. (11a) is the most natural. Keller [13] and Pennline [14] made several observations concerning accelerating the convergence rate associated with a successive approximation method for solving boundary value problems (or equivalently Fredholm integral equations).

Let us consider writing Eq. (11a) as

$$\frac{d^2\Theta}{d\eta^2}(\eta) - 4\beta^2\Theta(\eta) = \beta^2\Theta^4(\eta) - 4\beta^2\Theta(\eta), \quad \eta \in (-1,1), \quad (23)$$

where the coefficient on $\Theta(\eta)$ came about from the Maximum Principle [8] and subject to the previously described boundary conditions. Defining the differential operator L as

$$L = \frac{d^2}{d\eta^2} - 4\beta^2$$

and inverting yields

$$\Theta(\eta) = f(\eta) - \beta^2 \int_{\eta_0}^1 H(\eta, \eta_0) [\Theta^4(\eta_0) - \Theta(\eta_0)] d\eta_0, \quad \eta \in [-1,1], \quad (24)$$

where the two-parts Green's function $H(\eta, \eta_0)$ is

$$H(\eta, \eta_0) = \begin{cases} \frac{\sinh[2\beta(1-\eta)]\sinh[2\beta(1+\eta_0)]}{2\beta\sinh[4\beta]}, & -1 \leq \eta_0 \leq \eta, \\ \frac{\sinh[2\beta(1+\eta)]\sinh[2\beta(1-\eta_0)]}{2\beta\sinh[4\beta]}, & \eta \leq \eta_0 \leq 1. \end{cases} \quad (25)$$

Defining

$$\Phi(\eta) = \Theta^4(\eta) - 4\Theta(\eta), \quad (26)$$

and substituting this definition for $\Phi(\eta)$ into Eq. (24) produces

$$\Theta(\eta) = f(\eta) - \beta^2 \int_{\eta_0}^1 H(\eta, \eta_0) \Phi(\eta_0) d\eta_0, \quad \eta \in [-1,1]. \quad (27)$$

Next, substitute Eq. (27) into the right-hand-side of Eq. (26) to get

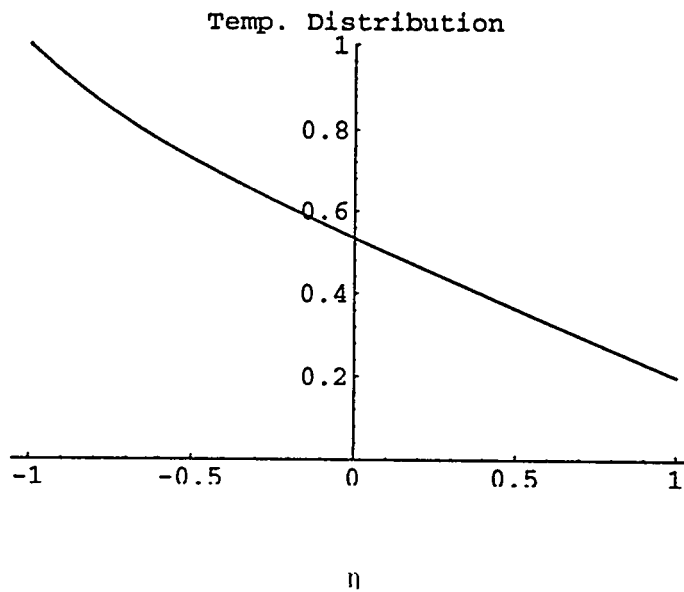
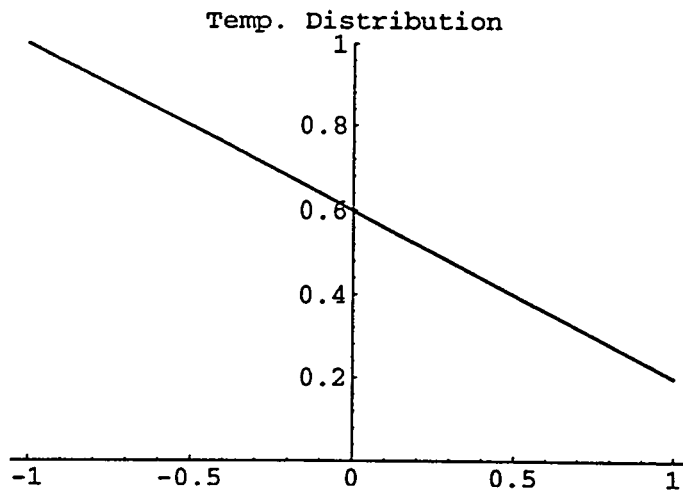


Figure 2. Temperature distributions $\theta_N(\eta)$ when $N = 5$ for
 a) $\beta = 0.1$ b) $\beta = 1$ when $\theta_2 = 0.2$.

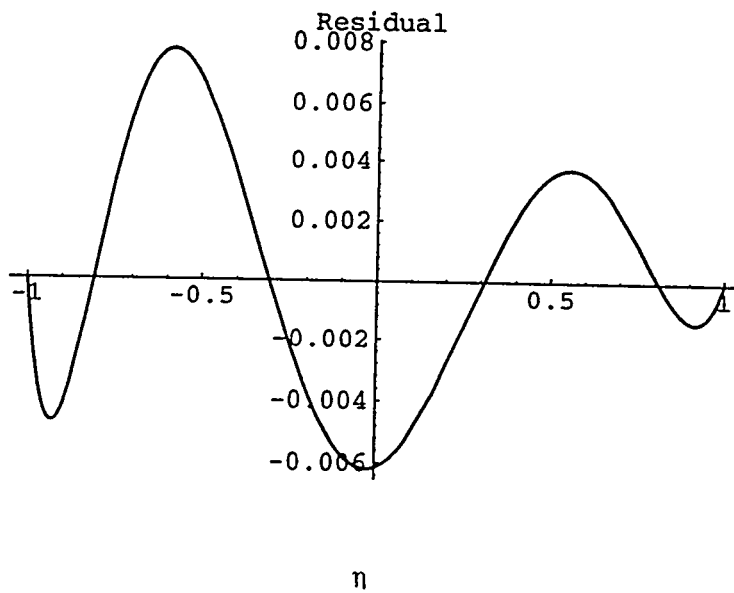
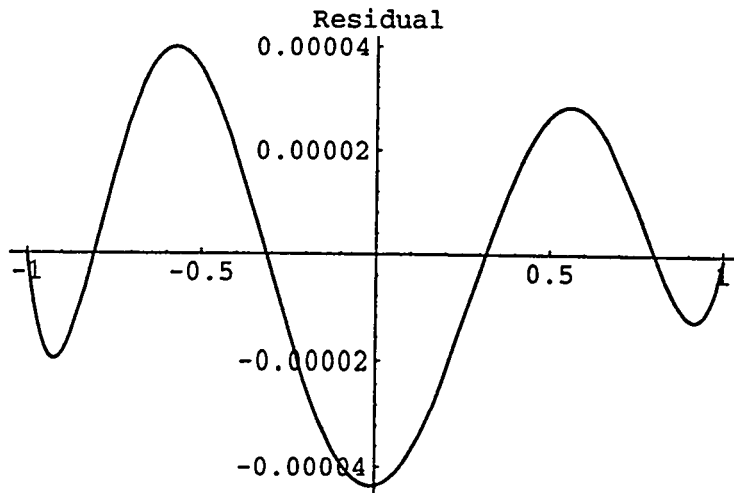


Figure 3. Residual distributions $R_x(\eta)$ when $N = 5$ for
 a) $\beta = 0.1$ b) $\beta = 1$ when $\theta_2 = 0.2$.

$$\begin{aligned} \Phi(\eta) = & [f(\eta) - \beta^2 \int_{\eta_0=-1}^1 H(\eta, \eta_0) \Phi(\eta_0) d\eta_0]^4 \\ & - 4[f(\eta) - \beta^2 \int_{\eta_0=-1}^1 H(\eta, \eta_0) \Phi(\eta_0) d\eta_0], \quad \eta \in [-1, 1]. \end{aligned} \quad (28)$$

As before, we represent the unknown function $\Phi(\eta)$ in terms of an infinite series, namely

$$\Phi(\eta) = \sum_{n=0}^{\infty} d_n^* T_n(\eta), \quad \eta \in [-1, 1], \quad (29)$$

or the approximation

$$\Phi_N(\eta) = \sum_{n=0}^N d_n^N T_n(\eta), \quad \eta \in [-1, 1]. \quad (30)$$

Introducing the approximation shown in Eq. (30) into Eq. (28) produces

$$\begin{aligned} R_N(\eta) = & - \sum_{n=0}^N d_n^N T_n(\eta) + [f(\eta) - \beta^2 \sum_{n=0}^N d_n^N C_n(\eta)]^4 \\ & - 4[f(\eta) - \beta^2 \sum_{n=0}^N d_n^N C_n(\eta)], \quad \eta \in [-1, 1]. \end{aligned} \quad (31)$$

Again, $C_n(\eta)$ is given by Eq. (19b). We can follow a similar procedure as outlined before in obtaining a system of nonlinear algebraic equations for the unknown expansion coefficients obtained by the collocation method. It is clear that this formulation will produce a higher operation count per iteration. However, it may converge substantially faster.

III. FUTURE PLANS AND CONCLUSIONS

The research is progressing quite rapidly. The main goals to be completed for the remaining portion of the first year were sighted in the previous section. The main objectives for the second year include:

- * To develop general (technically advanced) programs using Mathematica for solving the radiative equation of transfer and the energy equation using expansion methods.

- * To continue to consider and analyze error propagation, to develop appropriate error bounds, and to study convergence rates.

- * To expand the realm of problems to include an additional independent variable such as time, space or frequency (or equivalently wavelength). Each of these extensions have practical importance and could have substantial impact to several complicated energy-related problems of interest to DOE.

Appendix A:

Paper entitled: "Several Symbolic Augmented Cheyshev Expansions for Solving the Equation of Radiative Transfer" by J.I. Frankel, Ph.D. **Journal of Computational Physics**, (in review)

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Appendix B:

Paper entitled: "A Galerkin Solution to a Regularized Cauchy
Singular Integro-Differential Equation" by J.I. Frankel,
Ph.D., Quarterly of Applied Mathematics (accepted
for publication).

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Appendix C:

Paper entitled: "Generalization of the Method of Peters to Cauchy Singular Integro-Differential Equations", by J.I. Frankel, Ph.D., Proceedings of the Royal Society of London, Series A (in review).

Appendix C
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