

A CONVERSATIONAL EIGENANALYSIS PROGRAM FOR
SOLVING DIFFERENTIAL EQUATIONS^(a)

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ABSTRACT

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Dynamic models that arise in health physics applications are often expressed in terms of systems of ordinary differential equations. In many cases, such as box models that describe material exchange among reservoirs, the differential equations are linear with constant coefficients, and the analysis can be reduced to the examination of solutions of initial-value problems for such systems. This paper describes a conversational code, DIFSOL, that permits the user to specify the coefficient matrix and an initial vector of the system; DIFSOL prints out closed-form solutions [i.e., expressed as linear combinations of terms of the form e^{-at} , $e^{-at} \cos bt$, and $e^{-at} \sin bt$] and tables of the solution, its derivative, and its integral for any specified linear combination of state variables. The program logic permits menu-driven control. We have operated a FORTRAN IV version of the code on a DEC PDP-10 for several years. A translation into BASIC has proved practical on Radio Shack TRS-80 Model I and III personal computers for smaller systems of differential equations (<12 state variables). The paper includes illustrations of the use of DIFSOL in studying metabolic models.

MASTET

INTRODUCTION

Many of the dynamic/kinetic models used in health physics

research are formulated as systems of linear ordinary differential equations with constant coefficients. Examples are box models of material

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transfer among well-mixed compartments with constant transfer-rate coefficients (e.g., metabolic models of radionuclide uptake and removal from the body). Calibration and testing of such models frequently requires a computer program to permit efficient integration of the differential equations, and in many instances closed-form expressions for the solutions are needed.

The purpose of this paper is to describe such a program, DIFSOL, which has been in use for several years at Oak Ridge National Laboratory. DIFSOL exists in a conversational implementation for the Digital PDP-10 system, written in FORTRAN IV, and in a BASIC version for the Radio Shack TRS-80 Model I/III microcomputers. The program solves an initial-value problem of the form

$$\frac{dZ}{dt} = AZ, Z(0) = Z^0 \quad (1)$$

where Z is a vector of N functions, $Z_1(t), \dots, Z_N(t)$; A is a constant $N \times N$ coefficient matrix; and Z^0 is a constant vector of initial values for Z . The program uses matrix eigen-system analysis techniques to express the solution vector $Z(t)$ in terms of functions of the form e^{at} , $e^{at} \cos bt$, and $e^{at} \sin bt$. Responding to prompting from the program, the user inputs the matrix A and the initial vector Z^0 .

In this paper, we outline the method of solution used by DIFSOL and discuss three sample problems that illustrate its use. Finally, we indicate some practical limitations of the two versions of DIFSOL.

METHOD OF SOLUTION

In this section, we outline the matrix methods used to solve the system of differential equations given by Eq. 1.

We denote the N eigenvalues of A by W_j , $j = 1, \dots, N$. For each j , there is a corresponding eigenvector $R_j = [R_{1,j}, \dots, R_{N,j}]^T$, such that the pair W_j, R_j satisfies

$$AR_j = W_j R_j \quad (2)$$

Non-real eigenvalues of a real matrix A occur in complex conjugate pairs. Thus if the complex eigenvalue $W_j = \lambda_j + i\omega_j$ is such that $\omega_j \neq 0$, then $W_{j+1} = \lambda_j - i\omega_j$ is also an eigenvalue of A . We will assume that the eigenvalues have been indexed so that such complex conjugate pairs occur with successive indices: $W_{j+1} = \bar{W}_j$, where the bar represents the operation of taking the complex conjugate. The eigenvectors belonging to a complex conjugate pair of eigenvalues can be normalized so that they too are complex conjugates: $R_{j+1} = \bar{R}_j$. We shall assume in all that follows that this normalization has been accomplished.

A major assumption that we make is that the eigenvectors R_1, \dots, R_N form a linearly independent set. There are circumstances in which this assumption can be violated in practical problems, and when it is violated, DIFSOL will fail; but in such cases it is often possible to introduce small perturbations in the

parameters such that the perturbed system has linearly independent eigenvectors and its solution contains only second-order errors. Given the assumption, we see that Eq. 2 implies the existence of a diagonal matrix D , whose diagonal entries are just W_1, \dots, W_N , such that

$$AR = RD, \quad (3)$$

where $R = [R_1, \dots, R_N]$; this notation means that the columns of the matrix R are the N linearly independent eigenvectors of A . We conclude that R has an inverse, and hence the diagonal matrix D can be expressed as

$$D = R^{-1}AR. \quad (4)$$

We transform the system of Eq. 1 by introducing a new state vector $X = [X_1, \dots, X_n]^T$ as follows:

$$RX = Z, \quad (5)$$

so that the transformed system is found to be

$$\frac{d}{dt} X = DX, \quad X(0) = X^0, \quad (6)$$

where

$$X^0 = R^{-1}Z^0. \quad (7)$$

The system of Eq. 6 is uncoupled and can be solved in closed form by elementary methods. The relations of Eq. 5 and Eq. 7 can then be used to transform the solution vector X of the uncoupled system to the solution vector Z of the original coupled system. We indicate these steps in the

following paragraphs. We distinguish two cases.

Case 1

Eigenvalue W_j and eigenvector R_j are real. Then $W_j = \lambda_j$, and the j -th differential equation in the system defined by Eq. 5 is

$$\frac{dX_j}{dt} = \lambda_j X_j, \quad X_j(0) = X_j^0, \quad (8)$$

with solution

$$X_j(t) = \begin{cases} X_j^0 e^{\lambda_j t}, & \lambda_j \neq 0 \\ X_j^0, & \lambda_j = 0. \end{cases} \quad (9)$$

Case 2

Eigenvalues W_j and W_{j+1} are complex conjugate. The differential equations are

$$\frac{dX_j}{dt} = W_j X_j, \quad X_j(0) = X_j^0 \quad (10)$$

$$\frac{dX_{j+1}}{dt} = \bar{W}_j X_{j+1},$$

$$X_{j+1}(0) = X_{j+1}^0, \quad (11)$$

with solutions that can be written as follows:

$$X_j(t) = X_j^0 e^{W_j t} \quad (12)$$

$$x_{j+1}(t) = x_{j+1}^0 e^{\bar{W}_j t} \quad (13)$$

$$\begin{aligned} \text{where } |W_j|^2 &= |\bar{W}_j|^2 = W_j \bar{W}_j \\ &= \lambda_j^2 + \omega_j^2, \text{ and} \end{aligned}$$

$$e^{W_j t} = e^{\lambda_j t} (\cos \omega_j t + i \sin \omega_j t),$$

$$e^{\bar{W}_j t} = e^{\lambda_j t} (\cos \omega_j t - i \sin \omega_j t) = \overline{e^{W_j t}};$$

$$\text{also, } x_{j+1}^0 = \overline{x_j^0}. \text{ Hence } x_{j+1} = \bar{x}_j.$$

In transforming back to $Z = [Z_1, \dots, Z_N]^T$, using Eq. 5, we have

$$Z_s = \sum_{j=1}^N R_{s,j} x_j. \quad (14)$$

If indices j and $j+1$ correspond to a complex conjugate pair, their sum is a real quantity:

$$\begin{aligned} &R_{s,j} x_j + R_{s,j+1} x_{j+1} \\ &= R_{s,j} x_j + \bar{R}_{s,j} \bar{x}_j \\ &= R_{s,j} x_j + \overline{R_{s,j} x_j} \\ &= 2\Re(R_{s,j} x_j) \\ &= 2 \left\{ [\Re(R_j) \Re(x_j^0) - \Im(R_j) \Im(x_j^0)] \right. \\ &\quad \times e^{\lambda_j t} \cos \omega_j t \\ &\quad \left. - [\Re(R_j) \Im(x_j^0) + \Im(R_j) \Re(x_j^0)] \right. \\ &\quad \left. \times e^{\lambda_j t} \sin \omega_j t \right\} \quad (15) \end{aligned}$$

where $\Re(\)$ and $\Im(\)$ denote the real and imaginary part, respectively, of the parenthesized argument. Thus, in Eq. 14, pairs of complex conjugate terms, $R_{s,j} x_j$ and $R_{s,j+1} x_{j+1}$, can be replaced with corresponding pairs of real terms. Formally, we rewrite Eq. 14 as follows:

$$Z_s = \sum_{j=1}^N \rho_{s,j} \xi_j(t), \quad (16)$$

where $\rho_{s,j} = R_{s,j} x_j^0$ and $\xi_j(t) = e^{W_j t}$ if W_j is a real eigenvalue of A ; if j and $j+1$ are the indices of complex conjugate eigenvalues, then

$$\begin{aligned} \rho_{s,j} &= 2[\Re(R_j) \Re(x_j^0) - \Im(R_j) \Im(x_j^0)], \\ -\xi_j(t) &= e^{\lambda_j t} \cos \omega_j t, \end{aligned}$$

$$\begin{aligned} \rho_{s,j+1} &= -2[\Re(R_j) \Im(x_j^0) + \Im(R_j) \Re(x_j^0)], \\ \xi_{j+1}(t) &= e^{\lambda_j t} \sin \omega_j t. \end{aligned}$$

The following summary indicates the steps that DIFSOL is programmed to follow in solving the initial-value problem posed by Eq. 1.

1. Use eigenvalue/eigenvector routines to compute $W_j, R_j, j = 1, \dots, N$, for the real matrix A . Print and label the eigenvalues. If the eigenvectors R_j form a linearly dependent set, signal an error and stop.

2. Solve the linear algebraic system $RX^0 = Z^0$ for the vector X^0 . In general, this system must be assumed to have complex coefficients and requires a linear equation solving routine that works in complex arithmetic.

3. For $s = 1, \dots, N$, evaluate and print the coefficients $\rho_{s,j}$ of Eq. 16.

At the user's option, DIFSOL tabulates any specified linear combination of the solution functions $Z_s(t)$ at discrete times indicated by the user. The derivative and integral of the linear combination are also included in the tabulation.

The eigenvalue/eigenvector routines mentioned in Step 1 are from EISPACK (Smith et al., 1974); in the case of the microcomputer version of DIFSOL, these routines were translated from FORTRAN IV into BASIC. The routine for solving linear algebraic systems with complex coefficients is based on the real-arithmetic routines DECOMP and SOLVE (Forsythe et al., 1977) and consists of their application to a real system of size $2N$ derived from the original complex system of size N . Again, in the case of the microcomputer version, DECOMP and SOLVE were translated from their native FORTRAN IV into BASIC.

The matrix diagonalization that we have described above is a special case of a similarity transformation to a canonical form of the coefficient matrix (the Jordan canonical form is the one that is usually discussed in this connection). When the canonical matrix is diagonal, the diagonal entries are the eigenvalues of the coefficient matrix, and the eigenvectors are a linearly independent set; in these circumstances, we have the special case that we have described. When the set of eigenvectors of the matrix A is linearly dependent, the canonical matrix is not diagonal, and our method (and hence DIFSOL) fails. For discussion of the general case, we refer the reader to the literature. In parti-

cular, Gantmacher (1959) describes methods for the explicit computation of the transformation matrix. The application of the transformation to systems of ordinary differential equations with constant coefficients is treated by many authors; we cite Coddington and Levinson (1955), Petrovskii (1966), and Wilkinson (1965).

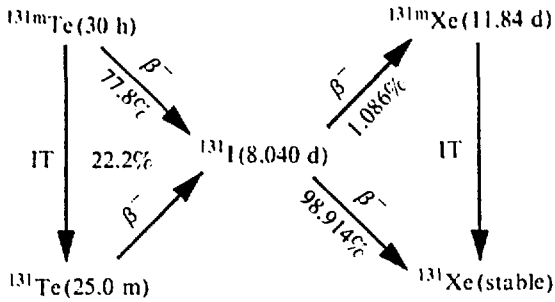
EXAMPLES

We give three examples to illustrate the form in which DIFSOL expects input and to show the interpretation of its output. We have rounded results to three and four figures to save space and make the examples easier to read.

Example 1. A Branching Radioactive Decay Chain

Figure 1 characterizes a portion of the radioactive decay chain that involves mass-number 131 isotopes of tellurium, iodine and xenon (Kocher, 1981). As an illustration of the use of DIFSOL, we assume that 1 Bq of ^{131m}Te is present initially, with zero amounts of the other species, and ask for the activity level of each of the four radionuclides as a function of time in days.

For $j = 1, \dots, 4$ (corresponding to ^{131m}Te , ^{131}Te , ^{131}I , and ^{131m}Xe , respectively) we write $\lambda_j^R = \ln(2)/T_j^R$, where T_j^R is the half-life of radionuclide j ; when the half-lives shown in Fig. 1 are converted to days, we calculate $\lambda_j^R = 5.55 \times 10^{-1}$, 3.99×10^{-1} , 8.62×10^{-2} , and $5.85 \times 10^{-2} \text{ day}^{-1}$, respectively. The differential equations are



Coefficient matrix A

$$\begin{bmatrix} -5.55 \times 10^{-1} & 0 & 0 & 0 \\ 8.86 & -3.99 \times 10^1 & 0 & 0 \\ 6.71 \times 10^{-2} & 8.62 \times 10^{-2} & -8.62 \times 10^{-2} & 0 \\ 0 & 0 & 6.35 \times 10^{-4} & -5.85 \times 10^{-2} \end{bmatrix}$$

FIGURE 1. Radioactive decay chain for mass-number 131 isotopes of tellurium, iodine, and xenon. The correspondence with compartment numbers in Example 1 is: $^{131m}\text{Te} - 1$; $^{131}\text{Te} - 2$; $^{131}\text{I} - 3$; and $^{131m}\text{Xe} - 4$.

$$\frac{dZ_1}{dt} = -\lambda_1^R Z_1$$

$$\frac{dZ_2}{dt} = \lambda_2^R (0.22Z_1) - \lambda_2^R Z_2$$

$$\frac{dZ_3}{dt} = \lambda_3^R (0.778Z_1 + Z_2) - \lambda_3^R Z_3$$

$$\frac{dZ_4}{dt} = \lambda_4^R (0.01086Z_3) - \lambda_4^R Z_4$$

with initial conditions $Z_1(0) = 1$, $Z_2(0) = Z_3(0) = Z_4(0) = 0$. The matrix A for this system is shown in Fig. 1. Table 1 gives the eigenvalues

(all of which are real) and the coefficients $\rho_{s,j}$ of Eq. 16. On the basis of this information, we may write the solutions as follows:

$$Z_1(t) = e^{-0.555t},$$

$$Z_2(t) = -0.225(e^{-39.9t} - e^{-0.555t}),$$

$$Z_3(t) = 0.184e^{-0.0862t} + 5 \times 10^{-4}e^{-39.9t} - 0.184e^{-0.555t},$$

$$Z_4(t) = 3.98 \times 10^{-3}e^{-0.0585t} - 4.22 \times 10^{-3}e^{-0.0362t} + 2.4 \times 10^{-4}e^{-0.555t}.$$

Example 2. Metabolic Model for Iodine

As a second example, we examine the metabolic model for iodine proposed by Riggs (1952) as adapted by the International Commission on Radiological Protection (ICRP) in ICRP Publication 30 Part 1 (ICRP, 1979) and Part 3, Addendum (ICRP, 1981). The latter reference defines the model as follows:

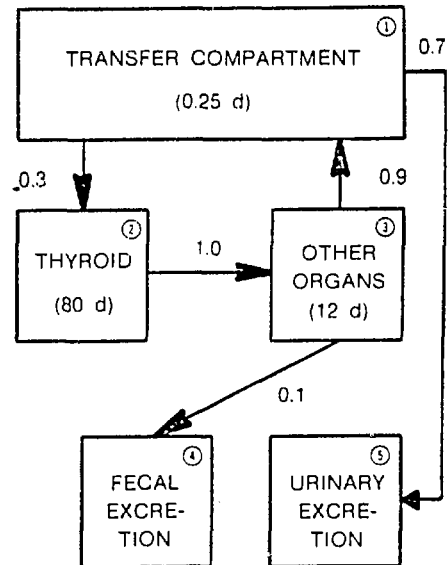
"Of iodine entering the transfer compartment a fraction fraction, 0.3, is assumed to be translocated to the thyroid while the remainder is assumed to go directly to excretion. Iodine in the thyroid is assumed to be retained with a biological half-life of 80 days and to be lost from the gland in the form of organic iodine. Organic iodine is assumed to be uniformly distributed among all organs and tissues of the body other than the thyroid and to be retained there with a biological half-life of 12 days. One-tenth of this organic

Table 1. Solution of Radioactive Decay Chain (Example 1): Eigenvalues and Coefficients

Eigenvalues	-5.85×10^{-2}	-8.62×10^{-2}	-3.99×10^1	-5.55×10^{-1}
Compartment				
1	0	0	0	1.00
2	0	0	-2.25×10^{-1}	2.25×10^{-1}
3	0	1.84×10^{-1}	4.88×10^{-4}	-1.85×10^{-1}
4	3.98×10^{-3}	-4.22×10^{-3}	-7.77×10^{-9}	2.36×10^{-4}

iodine is assumed to go directly to faecal excretion and the rest is assumed to be returned to the transfer compartment as inorganic iodine so that the effective half-life of iodine in the thyroid is 120 days."

A schematic of the model representing iodine metabolism in the transfer compartment, the thyroid, and all remaining organs and tissues is shown in Fig. 2. In addition, we have included compartments representing cumulative urinary and fecal excretion which are of interest in bioassay applications of the model. The inset table in Fig. 2 shows the nonzero entries of the coefficient matrix A that the user would input to DIFSOL. A non-zero initial condition of 1 unit is set for compartment 1,



NON-ZERO COEFFICIENTS OF THE MATRIX A

i	j	A_{ij}
1	1	$-\ln(2) \cdot 0.25 = -2.773$
2	1	$0.3 \ln(2) \cdot 0.25 = 0.832$
5	1	$0.7 \ln(2) \cdot 0.25 = 1.941$
2	2	$-\ln(2) \cdot 80 = -8.664 \times 10^{-3}$
3	2	$\ln(2) \cdot 80 = 8.664 \times 10^{-3}$
3	3	$-\ln(2) \cdot 12 = -5.776 \times 10^{-2}$
1	3	$0.9 \ln(2) \cdot 12 = 5.199 \times 10^{-2}$
4	3	$0.1 \ln(2) \cdot 12 = 5.770 \times 10^{-3}$

FIGURE 2. Compartment diagram for the model of iodine metabolism in the body proposed by Riggs (1952), with added compartments for cumulative urinary and fecal excretion (compartments 4 and 5). The non-zero entries of the matrix A are shown in the inset table.

Table 2. Solution of Iodine Metabolic Model (Example 2):
Eigenvalues and Coefficients

Eigenvalues	0	0	-6.04×10^{-2}	-6.04×10^{-3}	-2.77
Compartment					
1	0	0	-9.37×10^{-4}	9.00×10^{-4}	1.00
2	0	0	1.51×10^{-2}	2.86×10^{-1}	-3.01×10^{-1}
3	0	0	-4.89×10^{-2}	4.79×10^{-2}	9.60×10^{-4}
4	4.11×10^{-2}	0	4.67×10^{-3}	-4.57×10^{-2}	-2.00×10^{-6}
5	0	9.59×10^{-1}	3.01×10^{-2}	-2.89×10^{-1}	-7.00×10^{-1}

i.e., $Z_1^0 = 1$. The time constants and coefficients of the solutions are shown in Table 2.

In this example the zero eigenvalues correspond to constant terms (i.e., coefficient $\times e^{0t}$) in the solutions. Such terms appear in the solutions for compartments 4 and 5 (fecal and urinary excretion, respectively) because of the cumulative nature of these compartments. Thus, for example, the solution for compartment 5 is

$$\begin{aligned}
 Z_5(t) = & 0.9589 + 0.0301e^{-0.06043t} \\
 & - 0.2890e^{-0.0060t} \\
 & - 0.7000e^{-2.773t} .
 \end{aligned}$$

Example 3. Damped Harmonic Oscillator

To illustrate solutions with non-real eigenvalues, we turn to an example from classical mechanics and solve the equation

$$\frac{d^2\theta}{dt^2} + K \frac{d\theta}{dt} + \omega^2\theta = 0, \quad \theta(0) = 0,$$

$$\left. \frac{d\theta}{dt} \right|_{\theta=0} = 1, \quad (17)$$

where θ could be interpreted as the angular displacement of a simple pendulum which is constrained to small oscillations about $\theta = 0$. The first derivative term, with $K > 0$, represents a drag (e.g., air). To use DIFSOL, Eq. 17 must be represented as a first-order linear system, as follows: by setting $Z_1 = \theta$, $Z_2 = d\theta/dt$, we have

$$\frac{dZ_1}{dt} = Z_2$$

$$\frac{dZ_2}{dt} = -\omega^2 Z_1 - KZ_2.$$

We have taken $\omega = 2$ and $K = 0.5$ for this example. DIFSOL computer eigenvalues

$$W_1 = -0.25 + 1.984 i ,$$

$$W_2 = -0.25 - 1.984 i$$

and "compartment" coefficients $\rho_{1,1} = 0$, $\rho_{1,2} = 0.504$, $\rho_{2,1} = 1$, $\rho_{2,2} = -0.126$. The solutions are

$$Z_1(t) = 0.504e^{-0.25t} \sin 1.98t$$

$$Z_2(t) = e^{-0.25t} \times (\cos 1.98t - 0.126 \sin 1.98t),$$

and finally, $\theta(t) = Z_1(t)$. This concludes our presentation of examples.

DISCUSSION AND CONCLUDING REMARKS

The DIFSOL code was written several years ago at Oak Ridge National Laboratory as a tool for development and implementation of compartment models. Routines from EISPACK, a collection of state-of-the-art software for eigensystem analysis, form the core of the code. For implementation of DIFSOL on the authors' TRS-80 Model I and III microcomputers, the EISPACK routines were faithfully translated from FORTRAN IV into BASIC. Double precision arithmetic on the microcomputers (equivalent to about 16 decimal digits) is roughly comparable to that of the Digital PDP-10 system. The microcomputer implementation is usually practical for systems with fewer than, say, 12 equations; running times for the illustrative examples presented in this paper were less than five minutes.

We also need to point out that the method of solution employed in DIFSOL can encounter loss-of-significance difficulties, which, for some sets of data, can lead to quite meaningless results. This loss of significant digits arises when some of the terms in the sum of Eq. 15 are large in magnitude in comparison with the sum. When the disparity of magnitudes equals or exceeds the precision of the computation, the results are meaningless. Users of DIFSOL must be alert to this potential problem, which is inherent in the computational method and is not a quirk of the particular implementation. Used within its limitations, however, DIFSOL has proved to be an extremely valuable developmental tool.

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