NASA Technical Memorandum 84332

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March 1984

National Aeronautics and
Space Administration

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NUMERICAL MODELING OF D-MAPPINGS WITH APPLICATIONS TO CHEMICAL KINETICS

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Abstract. Numerical modeling of D-mappings has been studied and applied to solving nonlinear stiff systems. These mappings have been locally linearized for convergence analysis, and some applications have been made to chemical kinetics.

Keywords. Nonlinear equations; numerical methods; biomedical.

INTRODUCTION

A numerical method was developed by Dey (1977) for solving nonlinear systems, some applications of which were later made to stiff systems (Dey, 1982). Convergence analysis was done using nonlinear D-mappings (Dey, 1981).

It is extremely difficult to represent this analysis computationally. Local linearization for such an analysis, which rendered computational modeling of D-mappings feasible, was suggested by Lomax (1983). In this article we discuss linearized modeling of D-mappings and some applications of the method.

D-MATRICES AND D-MAPPINGS

If a sequence of square matrices of the same order satisfy the following condition,

$$\lim_{k\to\infty} A_k A_{k-1} \cdots A_1 = 0 \qquad (1)$$

each A_k is called a D-matrix. A D-matrix is not necessarily a convergent matrix, and conversely.

Theorem 1. A sufficient condition that A_k is a D-matrix is that

$$\|A_k\|_q \le \alpha < 1 \qquad (2)$$

$\forall\ k > K$ and that q is the same $\forall\ k$.

Theorem 1 is easily proved. Let

$$u^k = (u_1^k u_2^k \ \cdots\ u_J^k)^T \in D_k\ ,$$

$k = 1, 2, \ldots$, (u_j^k = value of u_j at some kth iteration).

Let us consider a chained linear spaces $D_k \subseteq D_{k-1} \subseteq \cdots \subseteq D \subset R^n$. R^n = n-dimensional real space. Let u^k, $u^* \in D_k\ \forall\ k$ and $G_k\colon D_{k+1} \times D_k \to D_{k+1}$. If

$$G_k(u^{k+1},u^k) - G_k(u^*,u^*)$$

$$= A_k(u^{k+1} - u^*) + B_k(u^k - u^*) \qquad (3)$$

and $\forall\ k > K$, and if $(I - A_k)^{-1}B_k$ is a D-matrix, G_k is called a D-mapping (Dey, 1981).

If we now consider a nonstationary iterative scheme of the form

$$u^{k+1} = G_k(u^{k+1},u^k) \qquad (4)$$

and if $G_k\colon D_{k+1} \times D_k \to D_{k+1}$ is a D-mapping, then

$$\lim_{k\to\infty} u^k = u^* \qquad (5)$$

where $u^* = G_k(u^*,u^*)\ \forall\ k$ (Dey, 1981).

LOCALLY LINEARIZED D-MAPPING

Let us linearize (4) on $D_k \times D_k$, using first-order approximation of $G_k(u^{k+1},u^k)$ near (u^k,u^k). Then,

$$u^{k+1} = G_k(u^k,u^k) + G_k'(u^{k+1} - u^k) \qquad (6)$$

where G_k' is the Fréchet derivative of G_k on $D_k \times D_k$. Equation (6) may be expressed as

$$u^{k+1} = A_k u^k + b_k \qquad (7)$$

where $A_k = -(I - G_k')^{-1}G_k'$, $b_k = (I - G_k')^{-1}G_k(u^k,u^k)$. We have assumed that $(I - G_k')$ is invertible. Now we may prove a second theorem.

Theorem 2. If (i) $|A_j - A^*| < E$, where E is a matrix consisting of elements that are positive and arbitrarily small and (ii) $|b_j - b^*| < \varepsilon$, ε is a vector consisting of elements that are positive and arbitrarily small, then (5) is true (convergence) if A_k is a D-matrix (Dey, 1983a).

Theorem 3. If G_k' is a D-matrix, so is A_k (Dey, 1983a).

This principle may now be applied computationally.

PERTURBED FUNCTIONAL ITERATION

Let a nonlinear system be expressed as

$$u = G_o(u) \tag{8}$$

$$u \in D, \quad G_o\colon D \to D$$

A Gauss-Seidel-type iteration for the solution may be expressed as

$$u^{k+1} = G(u^{k+1}, u^k) \tag{9}$$

$$G\colon D \times D \to D, \; u^k \in D \; \forall \; k$$

A perturbed iterative scheme (Dey, 1977) may be expressed as (in the element form)

$$u_j^{k+1} = \omega_j^{k+1} + G_j(u^{k+1}, u^k) \tag{10}$$

where

$$\omega_j^{k+1} = [G_j(G_j^{k+1,k}) - G_j^{k+1,k}] \times [1 - \partial_j G_j^{k+1,k}]^{-1} \tag{11a}$$

$$G_j^{k+1,k} = G_j(u_1^{k+1} \; . \; . \; . \; u_{j-1}^{k+1}, u_j^k \; . \; . \; . \; u_J^k) \tag{11b}$$

$$G_j(G_j^{k+1,k}) = G_j(u_1^{k+1} \; . \; . \; . \; u_{j-1}^{k+1}, G_j^{k+1,k}, u_{j+1}^k \; . \; . \; . \; u_J^k) \tag{11c}$$

$$\partial_j(G_j^{k+1,k}) = [\partial G_j/\partial u_j]_{u_1^{k+1}, u_2^{k+2} \; . \; . \; . \; u_{j-1}^{k+1}, G_j^{k+1,k}, u_{j+1}^k \; . \; . \; . \; u_J^k} \tag{11d}$$

The ω_j term is a perturbation parameter which accelerates the rate of convergence of (9) and stabilizes the numerical algorithm.

It has been proved (Dey, 1981) that if G is a D-mapping on $D_{k+1} \times D_k$, a necessary and sufficient condition for convergence is

$$\lim_{k\to\infty} |\omega_j^k| = 0 \; \forall \; j \tag{12}$$

Following Theorems 2 and 3 we may prove that if G_k' is a D-matrix, then (12) is true (linearized sense). Recent results (Dey, 1983b) using local linearization indicates that if

$$\max_{j,m} |G_{jm}| \le \beta/J \tag{13}$$

where $G_{jm} = \partial G_j/\partial u_m$ and $0 \le \beta < 1$, G in (9) is a D-mapping. In order that (13) may be correct, certain input parameters for the system (e.g., mesh size and time-step) have to be chosen in special ways. If this cannot be found a convex-type operation may be defined as follows:

$$\hat{G}_j(u,u) = (1 - \alpha_j)u_j + \alpha_j G_1(u,u) \tag{14}$$

Assuming $G_{jj}(u,u) \ne 1$, it has been found that $\hat{G}$ is a D-mapping (locally linearized) for the following:

1. $\alpha_j = (-1)^p(1 - G_{jj})^{-1}$ if $G_{jm} = 0$, $m \ne j$ and $p = 0$ if $G_{jj} < 1$, $p = 1$ if $G_{jj} > 1$.

2. $$\alpha_j = \min_{\substack{1 \le m \le j \\ m \ne j}} \left(\frac{\beta/J}{|G_{jm}|} \, , \; (-1)^p \frac{(1 + \beta/J)}{1 - G_{jj}} \right)$$

if $G_{jm} \ne 0$, $m \ne j$ and $p = 0$ if $G_{jj} < 1$, $p = 1$ if $G_{jj} > 1$. (15a)

where β is such that

$$1 > \beta \ge J\left(1 + \frac{|1 - G_{jj}|}{|G_{jm}|}\right)^{-1} \tag{15b}$$

3. $\alpha_j = 1$ if (13) is satisfied.

The algorithm of perturbed functional iteration including a linearized convergence analysis may be briefly expressed as follows. At each iteration level, compute G_{jm}, $m = 1, 2, \ldots, J$. If (13) is satisfied, set $\alpha_j = 1$; otherwise, compute α_j using (15). If $\alpha_j \ne 1$, replace G_j by $\hat{G}_j$, as given by (14). Compute ω_j using (11a)-(11d) and compute u_j at the new iteration level by (10). If (12) is satisfied at some iteration level, convergence is found; if $G_{jj} = 1$, the method fails.

In general, for a $J \times J$ system the method requires (i) $J^2 + J$ functionals to be computed for convergence analysis, (ii) partial linearization along the diagonal, and (iii) no Jacobians.

It has been proved analytically (Dey, 1977) that in the vicinity of the root, the method should display a superlinear rate of convergence.

A DEGENERATE IMPLICIT CODE

Let a nonlinear model be represented by

$$du/dt = f(u), \quad u = (u_1 u_2 \; . \; . \; . \; u_J)^T \tag{16}$$

$u(0) = u_0$ (initial condition). Approximating (16) by a two-point backward-difference scheme, we get:

$$u_j^{n+1} = u_j^n + \Delta t f_j(u^{n+1}), \; \Delta t = \text{time-step} \tag{17}$$

This nonlinear system may now be solved by the above method which forms a degenerate implicit code (since the one-step, matrix-inversion principle is not used for solution). If a convex-type operation of the form (14) is used, (16) becomes

$$du/dt = (I - \alpha)du/dt + \alpha f(u) \tag{18}$$

where $\alpha = \mathrm{diag}(\alpha_1, \alpha_2, \; . \; . \; . \; \alpha_J)$ and I = the identity matrix. If (16) is a stiff system, (condition number of $f'(u) >> 1$), it generally requires Δt to be very small if a functional iteration of the form (9) is applied for solution. In (18), α scales the elements in the Jacobian matrix $f'(u)$, and using (15) for α_j's mean (for a given Δt), D-mapping is found so that perturbed functional iteration converges.

APPLICATIONS

Application 1.

(Bui, 1979) $\mathring{u}_1 = -10{,}004\, u_1 + 10{,}000\, u_2^4$; $\mathring{u}_2 = u_1 - u_2 - u_2^4$; $u_1(0) = u_2(0) = 1$. An approximate solution is

$u_2(t) = \{10{,}004 \exp(-3t)/[10{,}008 - 4 \exp(-3t)]\}^{1/3}$

$u_1(t) = (10{,}000/10{,}004)u_2^4$. As $t \to \infty$, $u_1(t) \to 0$, $u_2(t) \to 0$. Linearizing this system near $u_1(0), u_2(0)$, the condition number is 10^4.

Using linearized convergence analysis for the degenerate implicit code we got $\Delta t \cong 10^{-5}$, a sufficient condition for convergence if $\alpha_j = 1$. Introducing (18) and computing α_j's in a subroutine using (15) we used $\Delta t = 10^{-3}$ to 10^8; correct results were found. No program interruption was cased. Details may be found in Dey (1983b).

Application 2. Irradiation of Neutral Water

The model developed by Chatterjee and Magee and the analysis of its numerical solution are given in Chatterjee and others (1983). The equations and the rate constants are given in Table 1. For our present analysis we linearized the system and computed α_j's. Stiffness was measured by Strate (1983) at t = 0, 0.1, 1, and 10. Condition numbers are, respectively, 10^{19}, 10^{12}, 10^{12}, 10^{10}(approximately). This may be seen to be true in Fig. 1. This pattern of solution was analyzed by Chatterjee and Magee and was found to be valid. Here, difference equations were formed by approximating the derivatives by using the two-point trapezoidal rule. D-mappings were introduced, and time-accurate solutions were computed with $\Delta t = 10^{-8}$, 10^{-6}.

CONCLUSION

Numerical solutions of stiff systems are generally obtained by using multistep implicit codes (Miranker, 1981) which require inversion of matrices obtained by computing Jacobians. This has been avoided in the technique explained here. However, the code is dependent on the Jacobians for its convergence analysis Such a linearized analysis seems to be quite effective, and, in contrast with its nonlinear counterpart, the complete analysis can be done computationally. More applications are under consideration.

ACKNOWLEDGMENT

I thank my 11-year-old son Charlie Dey for writing codes for the first problem in TRS-80 color computer.

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Table 1 Differential Equations for Transient Species and Radiation Products in Irradiated Neutral Water

$$
\begin{aligned}
\frac{d(H)}{dt} &= -2k_1(H)^2 - k_2(e^-_{Aq})(H) - k_5(H)(OH) + k_7(H_3O^+)(e^-_{Aq}) - k_9(H)(H_2O_2) \\
&\quad + k_{12}(OH)(H_2) - k_{13}(HO_2)(H) - k_{17}(H)(O_2) \qquad + 0.55\ I
\end{aligned}
$$

$$
\begin{aligned}
\frac{d}{dt}(e^-_{Aq}) &= -k_2(e^-_{Aq})(H) - 2k_3(e^-_{Aq})^2 - k_4(e^-_{Aq})(OH) - k_7(H_3\overset{+}{O})(e^-_{Aq}) \\
&\quad - k_{10}(e^-_{Aq})(H_2O_2) - k_{14}(e^-_{Aq})(O_2) \qquad + 2.65\ I
\end{aligned}
$$

$$
\begin{aligned}
\frac{d}{dt}(OH) &= -k_4(e^-_{Aq})(OH) - k_5(H)(OH) - 2k_6(OH)^2 + k_9(H)(H_2O_2) + k_{10}(e^-_{Aq})(H_2O_2) \\
&\quad - k_{11}(OH)(H_2O_2) - k_{12}(OH)(H_2) - k_{15}(HO_2)(OH) \qquad + 2.70\ I
\end{aligned}
$$

$$
\frac{d}{dt}(H_3^+O) = -k_7(H_3\overset{+}{O})(e^-_{Aq}) - k_8(H_3O^+)(OH^-) - k_{18}(H_3\overset{+}{O})(O_2^-) + k_{19}(H_2O) + k_{20}(HO_2) \qquad + 2\ 65\ I
$$

$$
\begin{aligned}
\frac{d}{dt}(H_2O) &= k_5(H)(OH) + k_8(H_3\overset{+}{O})(OH^-) + k_9(H)(H_2O_2) + k_{11}(OH)(H_2O_2) + k_{12}(OH)(H_2) \\
&\quad + k_{15}(HO_2)(OH) + k_{18}(H_3\overset{+}{O})(O_2^-) - k_{19}(H_2O) \qquad - 4.10\ I
\end{aligned}
$$

$$
\frac{d}{dt}(H_2) = k_1(H)^2 + k_2(e^-_{Aq})(H) + k_3(e^-_{Aq})^2 - k_{12}(OH)(H_2) \qquad + 0.45\ I
$$

$$
\begin{aligned}
\frac{d}{dt}(H_2O_2) &= k_6(OH)^2 - k_9(H)(H_2O_2) - k_{10}(e^-_{Aq})H_2O_2) - k_{11}(OH)(H_2O_2) + k_{13}(HO_2)(H) \\
&\quad + k_{16}(HO_2)^2 \qquad + 0.70\ I
\end{aligned}
$$

$$
\begin{aligned}
\frac{d}{dt}(OH^-) &= k_2(e^-_{Aq})(H) + 2k_3(e^-_{Aq})^2 + k_4(e^-_{Aq})(OH) - k_8(H_3\overset{+}{O})(OH^-) \\
&\quad + k_{10}(e^-_{Aq})(H_2O_2) + k_{19}(H_2O)
\end{aligned}
$$

$$
\begin{aligned}
\frac{d}{dt}(HO_2) &= k_{11}(OH)(H_2O_2) - k_{13}(HO_2)(H) - k_{15}(HO_2)(OH) - 2k_{16}(HO_2)^2 + k_{17}(H)(O_2) \\
&\quad + k_{18}(H_3\overset{+}{O})(O_2^-) - k_{20}(HO_2)
\end{aligned}
$$

$$
\frac{d}{dt}(O_2) = -k_{14}(e^-_{Aq})(O_2) + k_{15}(HO_2)(OH) + k_{16}(HO_2)^2 - k_{17}(H)(O_2)
$$

$$
\frac{d}{dt}(O_2^-) = k_{14}(e^-_{Aq})(O_2) - k_{18}(H_3\overset{+}{O})(O_2^-) + k_{20}(HO_2)
$$

where

$k_1 = 10^{10}$	$k_2 = 2.5\times10^{10}$	$k_3 = 6\times10^9$	$k_4 = 3\times10^{10}$
$k_5 = 2.4\times10^{10}$	$k_6 = 4\times10^9$	$k_7 = 2.3\times10^{10}$	$k_9 = 3\times10^{10}$
$k_9 = 10^8$	$k_{10} = 1.2\times10^{10}$	$k_{11} = 5\times10^7$	$k_{12} = 6\times10^7$
$k_{13} = 10^{10}$	$k_{14} = 1.9\times10^{10}$	$k_{15} = 10^{10}$	$k_{16} = 2\times10^6$
$k_{17} = 10^{10}$	$k_{18} = 3\times10^{10}$	$k_{19} = 5\ 5\times10^{-6}$	$k_{20} = 10^6$

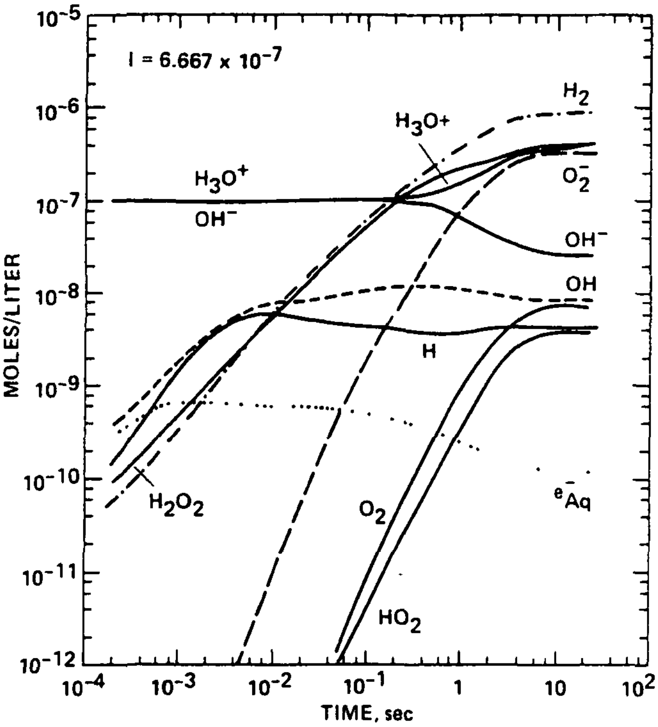

Fig. 1 Concentrations of species (Ex 2) vs. time for $I = 6.667 \times 10^{-7}$ in the logarithmic scale up to $t = 30$ sec. (Here steady state is reached for all the species.)

1 Report No	2 Government Accession No	3 Recipient's Catalog No
NASA TM-84332		

4 Title and Subtitle	5 Report Date
NUMERICAL MODELING OF D-MAPPINGS WITH APPLICATIONS TO CHEMICAL KINETICS	March 1984
	6 Performing Organization Code
7 Author(s)	8 Performing Organization Report No
S. K. Dey	A-9256
	10 Work Unit No
9 Performing Organization Name and Address	T-6469
Ames Research Center Moffett Field, CA 94035	11 Contract or Grant No
	13 Type of Report and Period Covered
12 Sponsoring Agency Name and Address	Technical Memorandum
National Aeronautics and Space Administration Washington, DC 20546	14 Sponsoring Agency Code

15 Supplementary Notes

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16 Abstract

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17 Key Words (Suggested by Author(s))	18 Distribution Statement
Nonlinear equations Numerical methods Biomedical	Unlimited Subject category - 64

19 Security Classif (of this report)	20 Security Classif (of this page)	21 No of Pages	22 Price*
Unclassified	Unclassified	8	A02

*For sale by the National Technical Information Service, Springfield, Virginia 22161