Convergence Promotion in the Simulation of Chemical Processes—The General Dominant Eigenvalue Method

The objective of this study was to devise an improved method of accelerating the iterative computation of steady state simulations of chemical processes. An extension of the dominant eigenvalue method is presented and its effectiveness is tested with simulations of chemical processes. The method is compared to previously available methods and is found to achieve convergence more rapidly and indeed was effective in cases where some other methods were ineffective or did not take a promotion step at all. The proposed method is applicable to the acceleration of any iterative computation of a nonlinear fixed-point problem.

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SCOPE

In the computer simulation of steady state chemical processes, iterative calculations must be carried out whenever the models are nonlinear and there are recycle streams. If the recycle computation is done sequentially, that is, the individual process units are computed one after another, one must guess starting values for the variables in some suitable set of streams, called *cut streams*. Each iteration then starts with a set of guessed values of cut variables x_n in the cut streams and produces a set of calculated values y_n. The next iteration starts with a new guess x_{n+1} obtained from previous values of x and y.

The iteration is said to have converged to a solution if the guessed and calculated values of the cut variables agree to within some specified tolerance. Unfortunately the achievement of convergence is often very slow so that there is a decided advantage in having an automatic means of accelerating progress toward the solution.

The previously available methods of convergence promotion have various limitations. Aitken's method (1925) is applied only to single variables, and later modifications by Wegstein (1958), Kliesch (1967), and Graves (1972) handle multivariable problems by treating each variable separately. Other methods for multivariable problems (Henrici, 1964) require generation, storage, and inversion of a large matrix. The dominant eigenvalue method (DEM) of Orbach and Crowe (1971) was effective for multivariable problems, but the possibility of extending DEM to using two or more dominant eigenvalues appeared to offer even more effective promotion of convergence. Crowe et al. (1971) have given an elementary discussion of convergence problems.

This paper proposes a new method of convergence promotion, called *general dominant eigenvalue method* (GDEM) which is an extension of DEM and which offers flexibility of use and more effective promotion steps.

The theoretical development of the general dominant eigenvalue method (GDEM) is presented, and it is compared with other available methods on two example problems, Cavett's flash problem and a simulation of the Bayer alumina process.

While the proposed method was developed to promote the convergence of chemical process simulations, it can be applied to other problems involving slowly converging iteration. Examples of such problems are sets of nonlinear equations which arise from finite difference approximation of nonlinear partial differential equations or from multicomponent chemical and physical equilibrium calculations.

CONCLUSIONS AND SIGNIFICANCE

The proposed method of promoting the convergence, GDEM, of iterative computations has been derived and tested on two cases, namely the Cavett (1963) flash problem and a simulation of the Bayer alumina process. GDEM was found to be a significantly more effective promoter of convergence than Orbach and Crowe's original DEM (1971) and than the methods of Wegstein (1958) as modified by Kliesch (1967) and by Graves (1972).

GDEM can be incorporated in a computer executive program for steady state simulation as a useful aid to attaining convergence and can be used independently of the structure of the specific process under study. GDEM also has a potential use in other iterative computations which involve nonlinear algebraic equations and which are slow to converge.

Many problems in chemical engineering, as well as in many other fields, must be solved numerically by an iterative procedure involving simultaneous nonlinear equations. For example, the computations of the steady state material and energy balance of a chemical process and the solution of nonlinear partial differential equations both require iteration.

Unfortunately, the convergence of the iterative procedure is often unacceptably slow so that some means of acceleration to promote convergence is desirable. Previous methods of convergence promotion include Aitken's method (1925), later adapted by Wegstein (1958), which was pri-

marily designed for single-variable problems and which ignores interaction between variables when used for multivariable problems. Wegstein's method has been further adapted by Kliesch (1967) and Graves (1972) who placed bounds on the promotion step which is taken but still did not account for interaction between variables. Aitken's method has been generalized for systems of m variables by Henrici (1964), but the extension requires the storage and inversion of an $(m \times m)$ matrix and a delay of m iterations before its use.

Orbach and Crowe (1971) described a technique for convergence promotion in multivariable problems, called the *dominant eigenvalue method* (DEM), which produced substantial reductions in the computation time of specific cases. DEM is an extension and application of the method of Lyusternik (1947), which was originally used in the numerical solution of partial differential equations. The purpose of this paper is to present a more general method of convergence promotion, which is more powerful than DEM, of which the DEM is a particular case, and which avoids the necessity of storage and inversion of large matrices. The basis of the new method is to assume that the iterations approximately follow a linear matrix difference equation and to compute the apparent solution by using estimates of products of the dominant eigenvalues.

DERIVATION OF THE PROCEDURE

Consider a problem involving iterative solution, such as typically arises in chemical engineering process calculations, where we wish to find a vector such that starting the calculations with it leads to exactly the same vector as the result. Such a problem can be regarded formally as one of finding the solution of

$$\mathbf{x} = \mathbf{f}(\mathbf{x}); \quad \mathbf{x} \in D \subseteq H \tag{1}$$

$\mathbf{f}$: $D \rightarrow D$ is assumed to be a continuous transformation, which may not necessarily be available explicitly but perhaps only in the form of a computer program. In the iterative computation of a chemical process, $\mathbf{x}$ represents the vector of guessed, or cut, variables and $\mathbf{f}$ is the computational algorithm which when applied to $\mathbf{x}$ produces a vector of calculated variables generally different from $\mathbf{x}$, unless the solution has been found. The general problem of solving simultaneous nonlinear algebraic equations can be also cast in the form of Equation (1). The norm defined on the space H is used in the development below to provide a measure of distance when testing for convergence.

It is usually not possible in practice to establish a priori the existence and uniqueness of a solution to Equation (1) in D, unless, for example, $\mathbf{f}$ can be shown to be a contraction mapping on a convex subset of D. It is normally assumed that the solution exists and—until more than one is found—that it is unique.

To find a solution to Equation (1) by computer, an iterative procedure of the form

$$\mathbf{y}_n = \mathbf{f}(\mathbf{x}_n) \quad (n = 0, 1, 2, \ldots)\ \mathbf{x}_0 \text{ specified} \tag{2a}$$

$$\mathbf{x}_{n+1} = \mathbf{x}_n + \mathbf{G}_n (\mathbf{y}_n - \mathbf{x}_n) \tag{2b}$$

is usually followed, generating a sequence $\{\mathbf{x}_n\}$ whose limit is assumed to exist in D. Here $\mathbf{G}_n$ is a forcing operator, normally linear and usually independent of iteration number n. One example is

$$\mathbf{G} = (1 + \alpha)\,\mathbf{I} \tag{3}$$

where α is a real number and $\mathbf{I}$ is the identity operator. For $\alpha = 0$, this is direct substitution, but a value $\alpha \neq 0$ may be found in some cases to improve the basic rate of convergence or to convert an unstable iteration into a stable one. Shacham and Motard (1974) recently discussed the effect of choosing different values of α. $\mathbf{G}$ may also be the appropriate constant Jacobian inverse for the modified Newton method. The proposed method which follows can be used to accelerate the convergence of any iterative procedure of the form (2) which is repeatedly applied, or indeed to any sequence of vectors which has a limit, provided that the convergence is ultimately linear. Thus, the method cannot be used with vector sequences generated by Newton's method which has quadratic convergence.

The basic hypothesis of the acceleration procedure is that the iteration can be approximated eventually by a linear difference equation:

$$\Delta\mathbf{x}_n = \mathbf{A}\,\Delta\mathbf{x}_{n-1} \tag{4}$$

where Δ is the forward difference operator. $\mathbf{A}$ is a linear operator which is not necessarily explicitly known, nor may the effort to evaluate it numerically be justified in general.

The characteristic equation for $\mathbf{A}$ can be written as

$$|\lambda\,\mathbf{I} - \mathbf{A}| = \sum_{j=0}^{m} \mu_j\,\lambda^{m-j} = 0 \tag{5}$$

where m is the dimension of the space H and the eigencoefficient μ_j,

$$\mu_j \equiv (-1)^j \sum \lambda_{i_1} \lambda_{i_2} \ldots \lambda_{i_j} \quad (1 \leq j \leq m)$$
$$1 \leq i_1 < i_2 \ldots < i_j \leq m \tag{6}$$

is the sum of all possible products of j of the m eigenvalues λ_l of $\mathbf{A}$. We define $\mu_0 \equiv 1$.

From the Cayley-Hamilton theorem (see Noble, 1969), $\mathbf{A}$ satisfies Equation (5) so that

$$\sum_{j=0}^{m} \mu_j\,\mathbf{A}^{m-j}\,\Delta\mathbf{x}_{n-m} = \mathbf{0} \tag{7}$$

and from repeated use of Equation (4),

$$\sum_{j=0}^{m} \mu_j\,\Delta\mathbf{x}_{n-j} = \mathbf{0} \quad (n \geq m) \tag{8}$$

It should be noted that Equation (8) is valid independently of whether eigenvalues are distinct or not and that the eigencoefficients μ_j are real even if some eigenvalues λ_l are complex.

Let the eigenvalues λ_j be labeled in descending order of absolute magnitude. Now let us suppose that only the first ν of them are large enough to dominate the iteration, in the sense that the iteration behaves essentially as if $\lambda_j \doteq 0$ $(j > \nu)$. Then it follows that

$$\sum_{j=\nu+1}^{m} \mu_j\,\Delta\mathbf{x}_{n-j} \doteq \mathbf{0} \tag{9}$$

since every term in Equation (6) for μ_j contains at least one λ_l $(j, l > \nu)$.

It may also be noted that the solution of Equation (4) may be written as

$$\Delta\mathbf{x}_n = \mathbf{A}^n\,\Delta\mathbf{x}_0 = \sum_{j=1}^{m} \mathbf{z}_j\,\lambda_j^n \tag{10}$$

with the $\mathbf{z}_j$ as eigenvectors of $\mathbf{A}$ if all λ_j are distinct.

If they are not distinct, Equation (10) must be modified, but in either case, as n becomes larger, terms in λ_j $(j > \nu)$ eventually become negligible relative to those with $j \leq \nu$, provided $|\lambda_\nu| > |\lambda_{\nu+1}|$. Then the iterations are essentially confined to a ν-dimensional subspace and approximation (9) can be adopted so that Equation (8) becomes

$$\sum_{j=0}^{\nu} \hat{\mu}_j \, \Delta \mathbf{x}_{i-j} \doteq 0 \quad (i = n, n+1, \ldots) \tag{11}$$

where $\hat{\mu}_j$ is an estimate of the true value μ_j and $\hat{\mu}_0 \equiv \mu_0 = 1$. It can then be said that the first ν eigenvalues are dominant.

Since Equation (11) cannot in general be exactly satisfied by any set of $\hat{\mu}_j$ when $\nu < m$, in order to be consistent with Equations (8) and (9) we estimate the coefficients μ_j so as to approach most closely to equality in Equation (11), namely,

$$\min_{(\mu_1, \mu_2, \ldots, \mu_\nu)} \left|\left| \sum_{j=0}^{\nu} \mu_j \, \Delta \mathbf{x}_{n-j} \right|\right|^2 \tag{12}$$

Here $||\cdot||$ is the norm defined on the space H. Since $\Delta \mathbf{x}_n \to 0$ as $n \to \infty$ when a solution exists, any norm (12) also $\to 0$. Usually one would choose either a Chebyshev (minimax) norm or one based on an inner product, such as a weighted sum of squares. Clearly whatever norm is selected increasing ν will in general improve the approximation (11) which will converge to exact equality as $\nu \to m$.

We used the inner product $\langle \cdot, \cdot \rangle$, defined in the space H as

$$\langle \mathbf{x}, \mathbf{y} \rangle \equiv \mathbf{x}^T \mathbf{W} \mathbf{y} \tag{13}$$

so that

$$||\mathbf{x}||^2 = \langle \mathbf{x}, \mathbf{x} \rangle \tag{14}$$

The matrix W would usually be the identity matrix or positive diagonal weighting matrix, with weights related to the inverse of the magnitude of the cut variables.

Then to estimate the μ_j, we take derivatives of the square norm (12) with respect to each μ_k and set them equal to zero, to obtain

$$\sum_{j=0}^{\nu} \hat{\mu}_j \, b_{jk} = 0 \quad (k = 1, 2, \ldots, \nu) \tag{15}$$

where

$$b_{jk} \equiv \langle \Delta \mathbf{x}_{n-j}, \Delta \mathbf{x}_{n-k} \rangle \tag{16}$$

Equation (15) can be solved numerically for the $\hat{\mu}_k$ by an efficient elimination technique for equations with a symmetric matrix.

At the end of iteration n, our object is to predict $\mathbf{x}_\infty$, the limit of the sequence $\{\mathbf{x}_n\}$ and to promote the attainment of convergence by starting the next iteration $(n+1)$ with an estimate of $\mathbf{x}_\infty$ instead of $\mathbf{x}_{n+1}$. Now by summing Equation (11) over i and interchanging the order of summation, we obtain

$$\hat{\mathbf{x}}_\infty - \mathbf{x}_{n+1} = \sum_{i=n+1}^{\infty} \Delta \mathbf{x}_i = - \sum_{j=1}^{\nu} \hat{\mu}_j \sum_{i=n+1}^{\infty} \Delta \mathbf{x}_{i-j} \tag{17}$$

Then by telescoping the right-hand summation, we find

$$\hat{\mathbf{x}}_\infty = \sum_{j=0}^{\nu} \hat{\mu}_j \, \mathbf{x}_{n+1-j} \Big/ \sum_{j=0}^{\nu} \hat{\mu}_j \tag{18}$$

Since we need $\Delta \mathbf{x}$ values for calculation of the $\hat{\mu}_j$, a more convenient form of Equation (18) is

$$\hat{\mathbf{x}}_\infty = \mathbf{x}_{n+1} - \left[\sum_{i=0}^{\nu-1} \left[\sum_{j=i+1}^{\nu} \hat{\mu}_j \right] \Delta \mathbf{x}_{n-i} \right] \Big/ \sum_{j=0}^{\nu} \hat{\mu}_j \tag{19}$$

It is worth noting that any promoter involving a finite linear combination of vectors, $\mathbf{x}_n, \mathbf{x}_{n-1}, \ldots$; as in Equation (18), should be an affine combination (that is, coefficients sum to unity) in order to guarantee that the estimated limit of a set of constant vectors is the constant vector itself.

Equation (19) provides convergence promotion of order ν and can be called the *general dominant eigenvalue method* (GDEM). An acceleration formula which is equivalent to Equation (19) was derived by Kovarik (1966) for a known linear operator A in a Banach space. A similar, but not equivalent, accelerator for iteration on linear equation systems has just been presented by Kaniel and Stein (1974). However, no comparison of their method with GDEM has been made.

In our studies, the order ν was usually fixed in advance and the estimated eigencoefficients $\hat{\mu}_j$ $(j = 1, 2, \ldots, \nu)$ were evaluated from Equation (15) at each iteration. In the original description of the DEM (Orbach and Crowe, 1971), a promotion step was taken when the estimates of the single dominant eigenvalue remained constant to within a prescribed tolerance. The obvious extension to several coefficients μ_j is to require that each one either remain substantially and separately constant, or be less than some small quantity. This was done initially but had the effect of making a promotion step the more infrequent, the greater was the number of μ_j evaluated. Indeed, it was observed that the estimates from Equation (19) of $\mathbf{x}_\infty$ on successive iterations could remain essentially constant despite quite wide variation in values of the $\hat{\mu}_j$.

Thus, the criterion for taking a promotion step which was finally adopted was to promote when estimates of the apparent solution $\hat{\mathbf{x}}_\infty^{(n)}$ at iteration n did not change more than a prescribed amount in the norm compared to the next prediction $\hat{\mathbf{x}}_\infty^{(n+1)}$, that is,

$$||\hat{\Delta \mathbf{x}}_\infty^{(n)}|| \,/\, ||\hat{\mathbf{x}}_\infty^{(n)}|| < \epsilon \tag{20}$$

or alternatively

$$||\Delta \chi|| < \epsilon \tag{21}$$

where

$$\Delta \chi_i \equiv \Delta \hat{x}_{\infty,i}^{(n)} / \hat{x}_{\infty,i}^{(n)}$$

If a promotion step is to be taken at iteration n, $\hat{\mathbf{x}}_\infty^{(n)}$ is usually used as the starting point for the next series of iterations. Each series would culminate in a convergence promotion step after some specified minimum number of iterations until finally convergence was achieved or the maximum number of iterations reached.

If $\nu = 1$, Equation (19) reduces to

$$\hat{\mathbf{x}}_\infty = \mathbf{x}_n + \Delta \mathbf{x}_n / (1 + \hat{\mu}_1) \tag{22}$$

which is the original dominant eigenvalue formula of Orbach and Crowe (1971) and for scalar x is Aitken's δ^2 formula (1926). The only difference is that here, using definition (16) and Equation (15)

$$\hat{\mu}_1 = - b_{01}/b_{11} \tag{23}$$

whereas Orbach and Crowe (1971) used

$$|\hat{\lambda}_1| = (b_{00}/b_{11})^{1/2} \tag{24}$$

together with a positive or negative sign for monotonic or oscillating convergence of elements of $\Delta \mathbf{x}$, respectively.

Thus, $\hat{\lambda}_1$ would correspond to $(-\hat{\mu}_1)$ in the present notation because of Equation (6).

From the Cauchy-Schwartz inequality,

$$|\hat{\mu}_1| \leq |\hat{\lambda}_1| \tag{25}$$

so that for the monotonic convergence ($\hat{\mu}_1 < 0$) the amount of promotion in Equation (22) is no greater using $\hat{\mu}_1$ rather than $(-\hat{\lambda}_1)$. This more conservative feature of the present method may avoid the necessity of taking only some fraction of the full promotion step, as was occasionally done by Orbach and Crowe (1971).

If $\nu = 2$, Equation (19) gives

$$\hat{\mathbf{x}}_\infty = \mathbf{x}_n + (\Delta\mathbf{x}_n - \hat{\mu}_2\,\Delta\mathbf{x}_{n-1})/(1 + \hat{\mu}_1 + \hat{\mu}_2) \tag{26}$$

where, from definition (16) and Equation (15)

$$\hat{\mu}_k = (b_{0i}\,b_{12} - b_{0k}\,b_{ii})/(b_{11}\,b_{22} - b_{12}^2); \quad (k = 1, 2 \text{ and } i = 3 - k) \tag{27}$$

If the Chebyshev norm is chosen, that is,

$$||\mathbf{x}||_\infty \equiv \operatorname*{Max}_i w_i\,|x_i| \tag{28}$$

where $\mathbf{w} > \mathbf{0}$, then analytical expressions for the coefficients $\hat{\mu}_j$ are not readily obtainable. They can, however, be computed for example by linear programming. Thus,

$$\operatorname*{Min}_{\boldsymbol{\mu}} \left|\left| \sum_{j=0}^{\nu} \mu_j\,\Delta\mathbf{x}_{n-j} \right|\right|_\infty \quad \text{with} \quad \mu_0 = 1 \tag{29}$$

is equivalent to Min ϵ
subject to

$$w_i\,|\Sigma\,\mu_j\,\Delta x_{n-j,i}| \leq \epsilon \quad (i = 1, 2, .., m) \tag{30}$$

It should be noted that the use of GDEM is not limited to a first-order matrix difference equation (4). If one wishes to use as a model

$$\Delta\mathbf{x}_n = \sum_{l=1}^{k} \mathbf{A}_l\,\Delta\mathbf{x}_{n-l} \tag{31}$$

this can be rewritten as a first-order difference equation

$$\Delta\mathbf{v}_n = \boldsymbol{\Gamma}\,\Delta\mathbf{v}_{n-1} \tag{32}$$

with

$$\mathbf{v}_n^T = [\mathbf{x}_n^T\ \mathbf{x}_{n-1}^T \ldots \mathbf{x}_{n-k+1}^T] \tag{33}$$

and

$$\boldsymbol{\Gamma} = \begin{vmatrix} \mathbf{A}_1 & \mathbf{A}_2 & \ldots & \mathbf{A}_k \\ I & 0 & \ldots & 0 \\ \cdot & I & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & & \cdot & \cdot \\ 0 & \ldots\ldots & I & 0 \end{vmatrix} \tag{34}$$

This is then of the same form as Equation (4) with the main difference that the prediction of $\mathbf{v}_\infty$ by Equation (19) would yield k estimates of $\mathbf{x}_\infty$.

TEST OF THE PROPOSED METHOD

The proposed method of convergence promotion, GDEM, was tested on two different steady state simulations, namely,

1. The well-known Cavett flash-tank problem (see Cavett, 1963; Henley and Rosen, 1969), which has two cut streams and 16 variables per stream.

2. The Bayer process for extraction of alumina from bauxite of Alcan Ltd., Arvida, Quebec. This simulation is described in a report to be published by Hoffman (1974). There were five cut streams and twenty cut variables per stream, in an information flow diagram with 86 streams and 47 equipment units. The iterations in each case were by direct substitution.

The effectiveness of the GDEM as a convergence promoter was compared with that of the Wegstein method as modified by Kliesch (1967), and by Graves (1972) using approximate constancy of the apparent solution as a criterion for promotion as shown in inequalities (20) or (21).

The results for the Cavett flash problem are shown in Figure 1 and Table 1. The original DEM and the present GDEM with $\nu = 1$ give the same results and are about as effective as any other GDEM promoter for this case. Graves' version of the Wegstein method was quite effective, but Kliesch's version was much less so. The GDEM with ν greater than one offered no clear advantage since the problem is easily converged, although $\nu = 7$ was slightly better than other values. It is seen that unpromoted iteration starts to oscillate after 63 iterations, probably as a result of interaction between iterative flash calculations inside the units and the overall iteration.

The results for the Bayer alumina process are shown in Table 2 and Figure 2. The estimation of the μ_j for GDEM was done using a diagonal weighting matrix W in Equation (13), whose elements were

$$W_{ii} = \text{Min}\ (0.0001,\ 1/x_i^2) \tag{35}$$

where x_i is a constant equal to the magnitude of the ith cut variable. This gave smoother results in this case than

Table 1. Cavett Flash Problem: Effect of Promoters on Convergence

Method	Total no. of iterations	No. of promotion steps	No. of iterations to reduce $\delta_n \leq \epsilon$ for $\epsilon =$ 1%	0.1%	0.01%	Final value of δ_n, %
No promotion	70	—	16	43	—	1.0×10^{-2}
Graves' method	44	1	16	25	39	8.2×10^{-3}
Kliesch's method	45	1	9	37	—	1.0×10^{-2}
GDEM, $\nu = 1$	24	5	7	15	21	8.4×10^{-4}
2	25	1	13	13	25	8.1×10^{-3}
3	21	3	8	14	17	9.7×10^{-4}
4	21	2	11	11	18	1.3×10^{-3}
5	20	2	11	11	19	3.5×10^{-4}
6	21	2	11	11	20	3.1×10^{-4}
7	16	1	12	12	12	1.3×10^{-3}
8	25	2	13	13	24	2.9×10^{-4}
9	21	1	14	14	18	7.3×10^{-3}
10	17	1	15	15	15	3.0×10^{-3}

TABLE 2. BAYER ALUMINA PROCESS: EFFECT OF PROMOTION ON CONVERGENCE

Method of promotion	Total no. of iterations	No. of promotions made	No. of iterations to first (last) reach $\delta_n < \epsilon =$ 10^{-3}	10^{-4}	10^{-5}	Final δ_n
No promotion	600*	—	2(2)	9(9)	216(216)	5.4×10^{-6}
Graves' method	326	1	2(2)	9(309)	216(—)	4.0×10^{-5}
GDEM, $\nu = 1$	400*	24	2(34)	9(396)	—	7.1×10^{-5}
3	190	10	2(2)	9(62)	88(188)	7.3×10^{-6}
4	169	8	2(2)	9(81)	—	1.6×10^{-5}
5	141	6	2(2)	9(71)	—	1.2×10^{-5}
6	118	5	2(2)	9(91)	62(112)	4.7×10^{-6}
7	199	8	2(2)	9(65)	110(183)	1.5×10^{-6}
8	133	2	2(2)	9(9)	133(133)	8.6×10^{-6}
9	153	5	2(2)	9(51)	81(153)	2.4×10^{-6}
10	119	3	2(2)	9(93)	111(111)	5.3×10^{-6}

* Maximum no. of iterations.

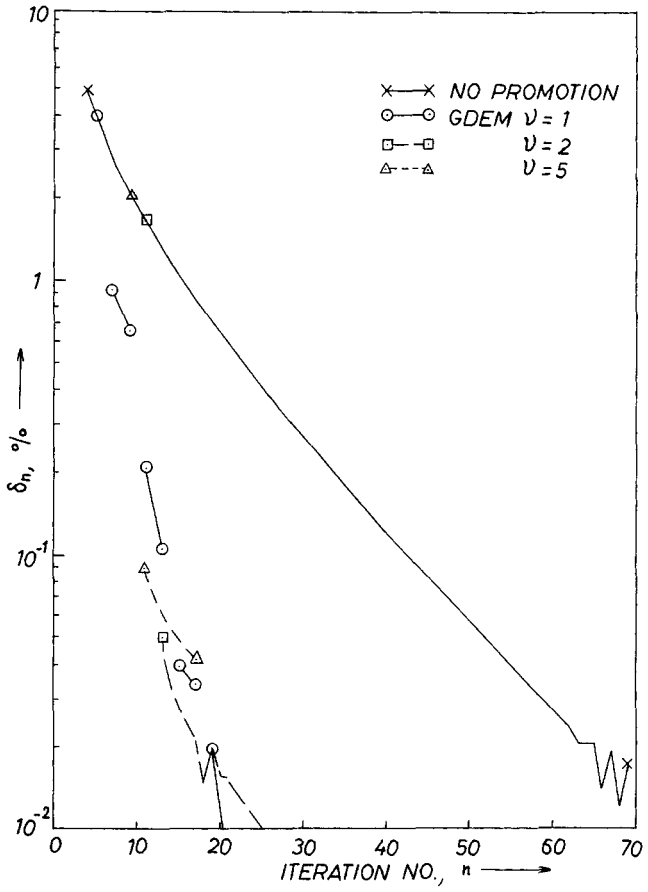

Fig. 1. Effect of promotion on iteration of Cavett flash problem: relative error δ_n vs. iteration number n.

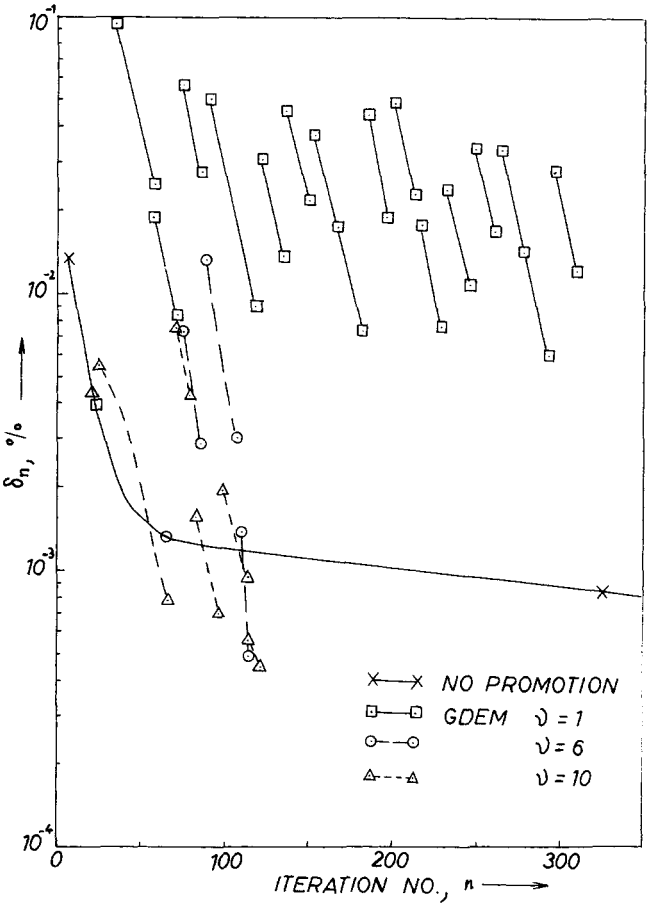

Fig. 2. Effect of promotion on iteration of Bayer process: relative error δ_n vs. iteration number n.

using equal weights for all cut variables. The progress of the computations was followed using

$$\delta_n = ||\Delta \mathbf{x}_n||_2 / ||\mathbf{x}_n||_2 \qquad (36)$$

to give a common basis for comparison of various convergence promoters. $||\cdot||_2$ is the norm (13) with $\mathbf{W} = \mathbf{I}$.

For the Bayer process, Kliesch's method was ineffective because no promotion steps were taken. Graves' method was somewhat unstable and only made one promotion step at iteration number 270. The GDEM was more effective and the best performance was obtained with $\nu = 6$ or 10. Indeed for $\nu = 1$, the GDEM was worse than using no promotion at all presumably because there are by computation several large eigenvalues very close together and to unit magnitude. Generally for larger values of ν there were fewer promotion steps taken, but the promotion was more effective. It is striking that the effectiveness of promotion does not monotonically increase with the value of ν. This can be explained by the fact that there were several pairs of complex eigenvalues with magnitudes close to unity. Any choice of ν which separates a pair of complex eigenvalues would violate the assumption that $|\lambda_\nu| > |\lambda_{\nu+1}|$, which leads to Equation (11).

One observes in Figure 2 that a promotion step was frequently taken when the slope of the graph was quite steep. Although this was not tried in these computations,

it would be useful to prevent a promotion step being taken while the iterations are proceeding fast enough without promotion, for example, when the ratio (δ_n/δ_{n+1}) exceeds some criterion $>> 1$.

If one wishes to choose the value of ν in advance for a problem which is to be computed many times with different data, the actual eigenvalues could be estimated by generating the matrix $\mathbf{A}$ to judge which μ_j should be negligible. Alternatively, one can carry out a computation without promotion and estimate μ_j in sets of one, two, three, and so on at each iteration in order to judge which if any of these sets becomes constant or, less stringently, which leads to more constant predictions of the apparent solution $\mathbf{x}_\infty^{(n)}$. The smaller ν is chosen to be the less storage and computation are required for promotion although the computation time required for promotion was relatively unimportant in comparison to the computation of the process itself.

The value of ν could also be selected automatically and continually during the computation so that approximation (11) is just satisfied to within a prescribed tolerance, that is,

$$\eta_1 \geqq \left|\left| \sum_{j=0}^{\nu} \hat{\mu}_j \, \Delta\mathbf{x}_{n-j} \right|\right| \geqq \eta_2 \geqq 0 \qquad (37)$$

where the norm is the same one used to estimate the $\hat{\mu}_j$. The value of ν would be increased by one if the upper bound was exceeded and decreased by one if the lower bound was passed. In tests on the Bayer process with $\eta_1 = 10^{-2}$, $\eta_2 = 10^{-4}$, no improvement over the best constant value of ν was achieved, but the results were certainly better than for $\nu = 1$.

It would seem preferable on theoretical grounds to use the same norm to follow the convergence as to estimate the μ_j. However, it is more important to use norms which behave smoothly so that the convergence will be achieved without erratic variation of the norm being followed.

CONCLUSION

A generally applicable procedure, GDEM, has been presented for accelerating the convergence of iterative calculations of the form of Equation (2). GDEM has been tested on two problems and found to provide more effective convergence promotion than other available methods. It is especially suitable for problems which are extremely slow to converge.

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NOTATION

$\mathbf{A}$ = $(m \times m)$ linearized iteration matrix, Equation (4)
b_{jk} = inner product, defined in Equation (16)
D = m-dimensional closed subset of H
$\mathbf{f}$ = continuous transformation: $D \rightarrow D$
$\mathbf{G}$ = forcing operator, Equation (2b)
H = any m-dimensional normed vector space
$\mathbf{I}$ = identity matrix
m = number of cut variables
n = number of iterations
$\mathbf{v}$ = block vector, Equation (33)
$\mathbf{w}$ = weighting vector, defined in Equation (28)
$\mathbf{W}$ = positive definite symmetric weighting matrix, Equation (13)
$\mathbf{x}_n$ = $(m \times 1)$ vector of guessed cut variables at iteration n
$\mathbf{y}_n$ = $(m \times 1)$ vector of calculated cut variables at iteration n
$\mathbf{z}_j$ = $(m \times 1)$ eigenvector of $\mathbf{A}$, for λ_j

Greek Letters

$\boldsymbol{\Gamma}$ = block matrix, Equation (34)
δ = ratio of norms, Equation (36)
Δ = forward difference operator
ϵ = small positive tolerance
$\eta_{1,2}$ = bounds on approximation (11) in Equation (37)
λ_j = jth eigenvalue of $\mathbf{A}$
μ_j = jth coefficient in characteristic polynomial of $\mathbf{A}$, Equation (6)
ν = number of coefficients $\hat{\mu}_j$ estimated, $\leqq m$

Subscript and Superscript

∞ = value at solution
$\wedge$ = estimated value

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