JOURNAL OF COMPUTATIONAL PHYSICS 103, 472–477 (1992)

NOTE

A Note on Compound Matrices

1. INTRODUCTION

The compound matrix method (CM) is essentially a clever adaptation of the shooting method for linear eigenvalue problems. Primitive shooting is notoriously unstable when applied to problems in which the target condition is computed from the solutions of the given system of differential equations in some multiplicative way, typically by the equations which must be generated from the original system. Thus the numerical error incurred in computing the target condition in an additive way but at the expense of solving a potentially much larger system of new differential equations which must be generated from the original system. Thus the numerical error incurred in computing the target value is only controlled by the accuracy with which the CM equations are solved. In a typical problem, the eigensystem is derived from the linearised form of the field equations and boundary conditions and thus is always homogeneous. In practice, two estimates of the critical eigenvalue are made for a given set of system parameters and these are used to generate target values by integrating the CM equations with a reputable library supplied routine. These two target values are now used as the genus of a secant convergence procedure whose objective is the determination of the eigenvalue for which the target value is zero, the iteration being terminated on a mixed error test. Note that the target value (generally complex) is an analytic function of the eigenvalue and it would be disadvantageous to treat the full problem in any way which countermanded this feature (e.g., by deliberately looking for purely imaginary eigenvalues for overstable modes). Without the analyticity property, complex secant convergence must be replaced by a more awkward beast. All results quoted in this note used a tolerance of 10^{-9} in the secant algorithm and the CM equations were integrated with NAG routine D02BAF and a tolerance of 10^{-9}. Computations were performed on an IBM3090.

Some early applications of the technique include work by Gilbert and Backus [1] in their discussion of elastic wave problems and work by Lakin *et al.* [2] to approximate the eigenvalues of the Orr–Sommerfeld problem. Ng and Reid [3] have extensively developed the method in their investigation of boundary layer and related stiff problems. Further details can be found in Drazin and Reid [4]. Recently an increasing number of applications have come from traditional applied mathematics. For example, Payne and Straughan [5] and Straughan [6] have fruitfully used the technique in linear and non-linear convective studies.

2. THE CONSTRUCTION PROCEDURE

We now consider a brief but rigorous account of the CM technique as it pertains to the boundary value problem

$$\begin{aligned} \frac{dY}{dz} &= A(\lambda, z)\, Y, \qquad z \in (0, 1) \\ BY &= 0 \qquad \text{on} \quad z = 0, \\ CY &= 0 \qquad \text{on} \quad z = 1, \end{aligned} \tag{2.1}$$

where λ is an eigenvalue, Y is an n vector, $A(\lambda, z)$ is an $n \times n$ matrix and B and C are respectively $(n-m) \times n$ and $m \times n$ matrices of full rank; i.e., $(n-m)$ conditions are given at $z=0$ and m conditions at $z=1$. We may assume without loss of generality that $m \leqslant n/2$. In Eqs. (2.1) λ, Y, A, B, and C are generally complex, but z is always real. All subsequent analysis is based on this assumption although in many important applications, the principle of exchange of stabilities is valid and the resulting eigenvalue problem can be formulated within a real framework effectively halving the number of CM equations. Let

$$\mathbf{y}_1(\lambda, z), \mathbf{y}_2(\lambda, z), ..., \mathbf{y}_m(\lambda, z)$$

be m linearly independent solutions of (2.1) each satisfying the boundary conditions at $z=0$ and define M to be the $n \times m$ matrix whose rth column is $\mathbf{y}_r(\lambda, z)$, i.e.,

$$M = [\mathbf{y}_1, \mathbf{y}_2, \mathbf{y}_3, ..., \mathbf{y}_m].$$

Equation (2.1) attributes M with the property

$$\frac{dM}{dz} = [A\mathbf{y}_1, ..., A\mathbf{y}_m] = AM. \tag{2.2}$$

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Any solution $\mathbf{W}(\lambda, z)$ of (2.1) satisfying the boundary conditions at $z=0$ has form

$$\mathbf{W}(\lambda, z)=\sum_{r=1}^{m} a_r \mathbf{y}_r(\lambda, z), \tag{2.3}$$

where $a_1, ..., a_m$ are complex constants not all identically zero. Since W must satisfy the boundary condition $CW=0$ at $z=1$ then

$$\sum_{r=1}^{m} a_r C\mathbf{y}_r(\lambda, z)=CM\mathbf{a}=\mathbf{0} \quad \text{on} \quad z=1 \tag{2.4}$$

in which $\mathbf{a}$ is the m vector whose rth component is a_r. Thus the $m\times m$ matrix CM is singular and this requirement determines acceptable λ values. In view of the Laplace expansion technique for the evaluation of determinants, it is obvious that

$$\det(CM)=\sum_{k=1}^{\binom{n}{m}} |C_k|\, \Phi_k, \tag{2.5}$$

where $|C_k|$ and Φ_k are $m\times m$ minors of C and M, respectively, and where the summation is performed over some exhaustive listing of the $\binom{n}{m}$ possible combinations of m rows of M out of n. Each compound matrix variable is defined to be a $m\times m$ minor of M in which the rows of M appear in increasing order, so this strategy can only succeed provided each variable can be evaluated at $z=1$. These values are obtained as the solution of an initial value problem.

The construction process begins with an exhaustive listing of all the possible minors of M. No unique enumeration scheme exists: within this work we shall enumerate each variable in terms of the m rows of M appearing in the determinant form and arranged in increasing order from left to right. Hence

$$\begin{aligned}
\Phi_1 &= (1, 2, 3, ..., m-1, m)\\
\Phi_2 &= (1, 2, 3, ..., m-1, m+1)\\
&\cdots\\
\Phi_{n-m+1} &= (1, 2, 3, ..., m-1, n)\\
\Phi_{n-m+2} &= (1, 2, 3, ..., m, m+1)\\
&\cdots\\
\Phi_{\binom{n}{m}} &= (n-m+1, ..., n-1, n),
\end{aligned} \tag{2.6}$$

where the general strategy is to systematically generate all variables containing the first row of M, then the second row of M, and so on until all possible combinations are realised. The differential equations satisfied by any Φ are constructed by observing that the derivative of this variable is a sum of m determinants in which the kth determinant has its kth row differentiated but the rest untouched. In view of (2.2), each differentiated row of M can be replaced by a linear combination of the rows of M and consequently each determinant in this sum can be expressed as a linear combination of the minors of M and hence as a linear combination of the other CM variables. In particular, coefficients appearing in this sum can be readily identified as entries of A. Thus the derivative of each variable is expressed as a sum of products involving an entry of A and a CM variable. In this way, $\binom{n}{m}$ differential equations are generated. The value of each variable at $z=1$ now is determined by integration of these equations with initial conditions that are consistent with the boundary condition at $z=0$.

By construction, M has rank m and so at least one of the CM variables is initially non-zero. Moreover, the remaining $(n-m)$ rows of M can be expressed as linear combinations of the m "preferred" rows and consequently the initial conditions exhibit one degree of freedom. Thus any set of initial conditions is equivalent to any other set modulo a constant multiplying factor. In practice, one of the non-zero variables is initialised to unity and the rest are automatically determined. Hence the target condition can be computed at $z=1$ as a linear combination of CM variables.

Clearly CM equations are eminently constructable by symbolic manipulation packages. We did not choose to use this route primarily because our objective was the construction of a utility which would take information from a control file and output a Fortran 77 subroutine characterising the specific application. The key to its operation lies in the observation that the entries of the original system matrix A are the coefficients appearing in the CM equations. All variables are constructed and differentiated symbolically within the utility but without the need for any external symbolic manipulation package. The CM strategy is now illustrated with a selection of examples from applied mathematics and physics.

3. BEAM OSCILLATIONS

The oscillation of a uniform beam in the absence of applied loads is governed by the non-dimensionalised equation

$$\frac{\partial^2 u}{\partial t^2}+\frac{\partial^4 u}{\partial z^4}=0 \qquad (z, t)\in(0, 1)\times(0, \infty) \tag{3.1}$$

in which $u(z, t)$ is the displacement of the beam at time t and position z. A normal modes analysis of (3.1) investigates solutions of type $u(z, t) = \mathrm{Re}(u(z)\, e^{i\omega t})$, where $u(z)$ satisfies the ordinary differential equation

$$\frac{d^4u}{dz^4} = \lambda u, \qquad z \in (0, 1), \quad \lambda = \omega^2.$$

This equation can be converted to the form $Y' = A(z, \lambda)\, Y$, where Y and A are respectively

$$Y = \left[u, \frac{du}{dz}, \frac{d^2u}{dz^2}, \frac{d^3u}{dz^3} \right], \qquad A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \lambda & 0 & 0 & 0 \end{bmatrix}. \tag{3.2}$$

Assuming that two boundary conditions are imposed at each of $z = 0$ and $z = 1$ then there are six compound matrix equations whose form only depends on (3.1). In terms of the variable enumeration scheme described in the construction procedure, the appropriate variables $\phi_1, ..., \phi_6$ may be represented by the abbreviated forms

$$\begin{aligned} \phi_1 &= (1, 2), & \phi_2 &= (1, 3), & \phi_3 &= (1, 4), \\ \phi_4 &= (2, 3), & \phi_5 &= (2, 4), & \phi_6 &= (3, 4), \end{aligned} \tag{3.3}$$

and satisfy the differential equations

$$\begin{aligned} \dot{\phi}_1 &= \phi_2, & \dot{\phi}_4 &= \phi_5, \\ \dot{\phi}_2 &= \phi_3 + \phi_4, & \dot{\phi}_5 &= -\lambda\phi_1 + \phi_6, \\ \dot{\phi}_3 &= \phi_5, & \dot{\phi}_6 &= -\lambda\phi_2. \end{aligned} \tag{3.4}$$

A variety of eigenvalue problems are possible for this beam but they are all generated from sensible combinations of the three types of end conditions portrayed by the mathematical requirements that either $u = u'' = 0$ (freely supported) or $u = u' = 0$ (cantilever supported) or $u'' = u''' = 0$ (unsupported). Every sensible combination yields real eigenvalues. The initial and target characterisations of these end conditions now follow:

End condition	Initial condition	Target condition
Free end	$\phi_5 = 1$, rest zero	$\phi_2 = 0$
Cantilever end	$\phi_6 = 1$, rest zero	$\phi_1 = 0$
Unsupported end	$\phi_1 = 1$, rest zero	$\phi_6 = 0$

Results are presented for the beam configurations Free–Free, Cantilever–Unsupported, and Cantilever–Free. In each of these cases it is easily verified that the corresponding natural frequencies, ω, satisfy respectively $\omega = n^2\pi^2$, $\cos\omega \cosh\omega = -1$, and $\tan\omega = \tanh\omega$. All computational timings are based on initial guesses which were in relative error by 10%:

Problem	Eigenvalue	True	Computed	CPU (s)
Free–Free	1st harmonic	97.40909	97.40906	0.141
	2nd harmonic	1558.5455	1558.5450	0.209
Cant–Unsup.	1st harmonic	12.36236	12.36236	0.112
	2nd harmonic	485.5188	485.5186	0.173
Cant.–Free	1st harmonic	237.72107	237.72097	0.148
	2nd harmonic	2496.4874	2496.4864	0.217

4. BENARD CONVECTION

The linear instability analysis for the convection of an incompressible viscous fluid contained between stationary boundaries $z = 0, 1$ requires the determination of the eigenvalues, σ, of the sixth-order system

$$\begin{aligned} \sigma(D^2 - a^2)w &= (D^2 - a^2)^2 w - Ra^2\theta, \\ \sigma P_r \theta &= (D^2 - a^2)\theta + Rw, \end{aligned} \tag{4.1}$$

where $D = d/dz$, w is the axial velocity component, θ is temperature, a is a wavenumber, P_r is the viscous Prandtl number and R^2 is the Rayleigh number. Typically boundaries are either stress free ($w = D^2w = 0$) or rigid ($w = Dw = 0$). In both cases the natural thermal condition has form $D\theta + h\theta = 0$, where h ($\geqslant 0$) is the Robin constant. For perfectly insulating boundaries, $h = 0$, whereas for perfectly conducting boundaries, h is very large and so $\theta = 0$. It is easily verified that (4.1) assumes the standard form $Y' = AY$, where

$$Y = \begin{bmatrix} w \\ Dw \\ D^2w \\ D^3w \\ \theta \\ D\theta \end{bmatrix}, \qquad A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -a^4 - \sigma a^2 & 0 & 2a^2 + \sigma & 0 & Ra^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ -R & 0 & 0 & 0 & a^2 + \sigma P_r & 0 \end{bmatrix}.$$

The principle of exchange of stabilities is valid for this problem and it can be easily verified that all eigenvalues are real. Only $\binom{6}{3} = 20$ CM equations are needed and their manual derivation is feasible. If $\phi_1, ..., \phi_{20}$ are the CM variables as enumerated in the construction procedure then they satisfy the differential equations

$$\begin{aligned}
\dot{\phi}_1 &= \phi_2 \\
\dot{\phi}_2 &= (2a^2+\sigma)\,\phi_1 + Ra^2\phi_3 + \phi_5 \\
\dot{\phi}_3 &= \phi_4 + \phi_6 \\
\dot{\phi}_4 &= (a^2+\sigma P_r)\,\phi_3 + \phi_7 \\
\dot{\phi}_5 &= Ra^2\phi_6 + \phi_{11} \\
\dot{\phi}_6 &= \phi_7 + \phi_8 + \phi_{12} \\
\dot{\phi}_7 &= (a^2+\sigma P_r)\,\phi_6 + \phi_9 + \phi_{13} \\
\dot{\phi}_8 &= (2a^2+\sigma)\,\phi_6 + \phi_9 + \phi_{14} \\
\dot{\phi}_9 &= (2a^2+\sigma)\,\phi_7 + (a^2+\sigma P_r)\,\phi_8 + Ra^2\phi_{10} + \phi_{15} \\
\dot{\phi}_{10} &= \phi_{16} \\
\dot{\phi}_{11} &= -(a^4+\sigma a^2)\,\phi_1 + Ra^2\phi_{12} \\
\dot{\phi}_{12} &= \phi_{13} + \phi_{14} \\
\dot{\phi}_{13} &= -R\phi_1 + (a^2+\sigma P_r)\,\phi_{12} + \phi_{15} \\
\dot{\phi}_{14} &= (a^4+\sigma a^2)\,\phi_3 + (2a^2+\sigma)\,\phi_{12} + \phi_{15} + \phi_{17} \\
\dot{\phi}_{15} &= -R\phi_2 + (a^4+\sigma a^2)\,\phi_4 + (2a^2+\sigma)\,\phi_{13} \\
&\quad + (a^2+\sigma P_r)\,\phi_{14} + Ra^2\phi_{16} + \phi_{18} \\
\dot{\phi}_{16} &= -R\phi_3 + \phi_{19} \\
\dot{\phi}_{17} &= (a^4+\sigma a^2)\,\phi_6 + \phi_{18} \\
\dot{\phi}_{18} &= -R\phi_5 + (a^4+\sigma a^2)\,\phi_7 + (a^2+\sigma P_r)\,\phi_{17} + Ra^2\phi_{19} \\
\dot{\phi}_{19} &= -R\phi_6 + \phi_{20} \\
\dot{\phi}_{20} &= -R\phi_8 - (a^4+\sigma a^2)\,\phi_{10} + (2a^2+\sigma)\,\phi_{19},
\end{aligned}$$

where σ is real. Initial and target properties of the CM variables pertaining to stress-free boundaries and rigid boundaries are

Boundary type	Initial condition	target condition
Stress-free	$\phi_{14}=1, \phi_{15}=-h$, Rest zero	$h\phi_6+\phi_7=0$
Rigid	$\phi_{17}=1, \phi_{18}=-h$, Rest zero	$h\phi_3+\phi_4=0$

For two stress-free conducting boundaries (i.e., $h=\infty$), the corresponding eigenvalue problem is characterised by the initial conditions $\phi_{15}=1$, rest zero, and the target condition $\phi_6=0$. It is well known that stationary instability (i.e., $\sigma=0$) occurs when $a \approx 2.221$ and $R^2 \approx 657.511$. Values for σ when $a=2.221$ and $P_r=1$ are given for selected R^2 values in the vicinity of $R^2=657$:

Rayleigh No. R^2	Computed eigenvalue σ	CPU (s)
645	−0.1415	0.329
650	−0.0848	0.329
655	−0.0283	0.330
660	+0.0280	0.329
665	+0.0841	0.331

Magnetohydrodynamic effects can be incorporated into Eqs. (4.1) and lead to the eighth-order system

$$\begin{aligned}
\sigma(D^2-a^2)w - \sigma P_m Db &= (D^2-a^2)^2 w \\
&\quad - Ra^2\theta - QD^2 w, \\
\sigma P_m b &= QDw + (D^2-a^2)b, \\
\sigma P_r \theta &= (D^2-a^2)\theta + Rw,
\end{aligned} \tag{4.2}$$

where D, w, θ, a, P_r, and R^2 have their previous meanings and b, P_m, Q are respectively the axial magnetic induction, the magnetic Prandtl number, and the Chandrasekhar number. Of course, mechanical and thermal boundary conditions must now be supplemented by a magnetic condition. It is common practice to associate stress-free with electrically insulating boundary conditions (i.e., $Db=0$) and to associate rigid with electrically perfectly conducting boundary conditions. Further system variables $y_7=b$ and $y_8=Db$ must be introduced, but within this extended framework, Eq. (4.2) is representable in the form $Y'=AY$, where A in now an 8×8 matrix.

Chandrasekhar [8] has studied Eqs. (4.2) and it is well known that overstable and stationary instability are both possible if $P_m > P_r$. Hence the critical eigenvalues of (4.2) can be complex although A is real. Since the boundary conditions are evenly split, $\binom{8}{4}=70$ complex or 140 real CM equations are needed. It is not profitable to present these equations here but in our opinion their formulation lies on the edge of manual credibility although the utility constructs a suitable Fortran subroutine almost instantly. Some appropriate initial and target conditions on CM variables are

Boundary type	Initial condition	Target condition
Stress-free electrically insulating	$\phi_{47}=1, \phi_{49}=-h$, $\phi_{117}=1, \phi_{119}=-h$, Rest zero	$h\phi_{22}+\phi_{24}=0$ $h\phi_{92}+\phi_{94}=0$
Rigid electrically conducting	$\phi_{58}=1, \phi_{60}=-h$, $\phi_{128}=1, \phi_{130}=-h$, Rest zero	$h\phi_{11}+\phi_{13}=0$ $h\phi_{81}+\phi_{83}=0$

where $\phi_n + i\phi_{n+70}$ is the nth complex CM variable. Some results for two stress-free, electrically insulating and thermally perfectly conducting boundaries are presented when $P_r = 1$, $P_m = 3$, and $Q = 100$. Chandrasekhar [8] proves that the threshold for stationary instability is independent of P_r and P_m. In fact,

$$a_{\text{over}} = 2.657 \qquad R^2_{\text{over}} = 1747.76,$$

$$a_{\text{stat}} = 3.702 \qquad R^2_{\text{stat}} = 2653.701.$$

Critical eigenvalues in the vicinity of the overstable mode are illustrated in the following table of results. All timings are based on initial guesses of $\sigma_1 = 9i$ and $\sigma_2 = 8.5i$ in the secant algorithm.

Rayleigh No. R^2	Eigenvalue σ	CPU (s)
1750	$0.00961 + i8.812$	3.534
1748	$0.00100 + i8.820$	3.535
1746	$-0.00763 + i8.829$	3.526
1744	$-0.01625 + i8.838$	3.533

5. CONCLUSIONS

We conclude with a summary of some major advantages and disadvantages of the compound matrix technique in connection with eigenvalue problems and contrast these with a comparable matrix method, say *inverse iteration.* Both aim to estimate the system eigenvalue closest to some initial guess and in this respect both methods require a reliable start.

Advantages

(1) The original boundary value problem is exactly converted into an equivalent initial value problem in contrast to matrix methods where an element of truncation takes place in the sense that the eigenfunction is either discretized or approximated by some finite series.

(2) The CM equations themselves are dependent only on the order of the original system and the split of the boundary conditions. Their specific nature only enters the problem through initial and target requirements and consequently sophisticated boundary conditions can be treated and amended with considerable ease. For example, in convection problems, it is often desirable to consider all combinations of free, rigid, and mixed boundaries in addition to a variety of thermal conditions. Such alterations are implemented by varying the initial and target requirements. In contrast, matrix methods tend to embed boundary conditions within the system matrix. Often it is possible to accommodate such changes with ease but we believe that this procedure is potentially more error-prone than the CM approach, especially with technically complicated boundary conditions.

(3) Matrix methods can be memory intensive. In contrast, CM methods rely on differential equation integrators which are often economical in memory requirements and so even large applications can be implemented on a microcomputer. Programme coding is usually straightforward once the system of controlling equations are constructed.

(4) Often matrix methods require a reasonable degree of mathematical competence, not only in the construction of the system matrix, but also in the development of the related software to analyse this matrix. Sometimes it is possible to convert the given system into a single differential equation with a corresponding simply banded matrix and, on such occassions, an "off the shelf" treatment can be employed. However, many recent applications involve systems with non-constant coefficients (often numerically determined) and, in such cases, the single high-order differential equation may not be a realistic possibility. For example, inverse iteration typically generates complex matrices which are block structured with banded non-zero blocks. To our knowledge such programme material cannot be regarded as "off the shelf." Indeed the solution of problems of this type are more akin to preconditioning and conjugate gradient methods. On the other hand, the CM method only requires a differential equation integrator and the performance of the technique is only limited by the quality of this integrator. All major software libraries have an abundance of high quality software in this department. Hence the CM approach offers the casual user high quality performance with minimal effort. In a non-stiff environment, an extrapolation integrator such as Stoer and Bulirsch [7] can be particularily effective.

(5) In many applications, the CM methods return a superior accuracy to matrix methods in view of the exactness of the procedure. For example, it is well known that the accuracy of inverse iteration deteriorates markedly if the system matrix is "too large." Although this is not regarded as serious, it is nevertheless disconcerting that such instabilities appear. No such difficulties arise with compound matrices.

Disadvantages

(1) It is difficult to extract the eigenfunction from the CM variables, whereas with matrix methods, the eigenfunction is often obtained directly as some high-dimensional vector or is approximated by some finite series. Drazin and Reid [4] show how this is done for the Orr–Sommerfeld equation.

(2) The equation generation process is often tedious and requires the generation of a sizeable number of first-

order differential equations. However, the procedure is routine and is eminently suited to automatic construction. We are happy to supply a well-tested utility to perform this operation and believe that its existence enhances the applicability of the technique (Email GAMA11 at UK.GLASGOW.CMS). In our opinion, the proliferation of equations becomes unacceptable for 12 or above (e.g., at order 12, as many as 924 equations may be required) and, although other methods are also becoming less manageable, they are likely to become more attractive as order increases. However, systems whose order exceeds 11 are regarded as unusual. As a matter of interest only m^2+1 of the $\binom{n}{m}$ compound matrix variables are independent; the rest of the equations are by-products of the algebraic structure inherent in the variable definitions.

(3) Whenever boundary conditions are unevenly distributed, the number of compound matrix variables is substantially reduced. However, in most applications the original system is even and the boundary data is evenly distributed and this is unfortunately the worst possible scenario.

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Received November 29, 1990; accepted April 14, 1992

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