A Minimization Method for Treating Convergence in Modal Synthesis

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The problem of convergence in modal synthesis is solved by a minimization approach. Substructure modes corresponding to fixed-interface boundaries are considered. The Rayleigh quotient of the structure is defined in a coordinate space which includes the initial selection of substructure modes augmented by some of the unused modes. It is scaled and projected onto a subspace orthogonal to the lower order modes. An unconstrained minimization problem is formulated for each mode using this function. Starting points correspond to eigenvectors obtained from the initial solution. The scaling transformation tends to point the vector of steepest descent toward the minimum. An optimum step in this direction provides a lower bound on the eigenvalue error and a corresponding estimate of eigenvector error. The magnitude of the gradient vector provides another measure of the truncation error. These are compared formally and by numerical example. For small errors, the Rayleigh quotient is minimized to first-order approximation by a single step consistent with small perturbation theory. For larger errors, the Conjugate Gradient algorithm is used to drive each mode to convergence in an iterative manner.

Introduction

MODAL synthesis is a Rayleigh-Ritz approach using systematically derived displacement functions. It is used to formulate and solve the large eigenproblems which arise in dynamic analyses of complex structural systems. Solutions are approximate in the sense that the motion of the structure is constrained to linear combinations of a limited number of modes or displacement functions characterizing the behavior of independent substructures. System modes derived in this way are said to have converged whenever relaxation of the modal constraints does not cause them to change appreciably. Two problems related to establishing convergence are frequently encountered after obtaining an initial solution: 1) to identify the modes within a frequency range of interest which have not converged; and 2) to find a suitable way of improving them.

Hurty[1,2] is credited with the initial development of a method which he calls component mode synthesis, applicable to redundantly connected substructures. Craig and Bampton[3] simplified Hurty's formulation by combining two groups of coordinate functions which Hurty had defined separately. Since then, several variations of modal synthesis have emerged. They are similar in concept but differ in the type of substructure modes used. Interface boundary conditions must be specified in order to obtain modal displacements independent of neighboring substructures. The boundary conditions may be fixed, free, or reflect some intermediate condition such as mass or stiffness loading. The common objective of these methods is to achieve a formulation which will permit an accurate representation of system motion with the fewest substructure modes. A number of recent survey papers have been written, including papers by Hou,[4] Hurty,[5] Hurty, Collins, and Hart[6] and Benfield, Bodley, and Moroso.[7] Some methods are found to be more suitable for certain applications than others. Yet, experience has shown that no single approach is generally preferred over the others. Hurty's method is one of the simplest and has demonstrated good convergence properties. It has been widely accepted and is chosen as the basis for the present work.

There appears to be no way of making an a priori selection of substructure mode coordinates which guarantees the convergence of system modes over a predetermined range of frequencies. To do so would require some knowledge of the outcome beforehand. In the absence of such knowledge, one is forced to make his selection on the basis of previous experience and to evaluate his results afterward. Hurty[5,8] has derived a measure of eigenvalue error based on a linear perturbation of the initial solution. Bajan, Feng, and Jaszlics[9] have derived a similar expression which they have used in an automated procedure to evaluate the relative importance of the unused modes and introduce them sequentially into a procedure which converges upon the unconstrained system modes. This method requires several eigenproblems solutions of the same size as the original one. Even though most of the system modes may be convergent after the initial solution, this approach requires that all of them be resolved in each iteration. By contrast, the method developed here requires that only the nonconvergent modes be re-evaluated.

In the following paragraphs, a form of the Rayleigh quotient for a structural system is derived, such that when subjected to direct minimization, it yields one of the eigenvalues of the coupled system. Several coordinate transformations are introduced. The Rayleigh quotient is initially defined in an expanded component mode coordinate space. The initial set of component mode coordinates is transformed to the set of system modes derived in the original solution. A mixed coordinate system results which includes both system and component-type modes. A scaling transformation is derived to numerically balance these equations. Finally, in order to allow the minimization to converge to a higher order mode, a transformation is derived to project the scaled Rayleigh quotient onto a subspace which is orthogonal to the lower order modes. The procedure lends itself to physical interpretation as well as mathematical convenience.

Modal Synthesis Formulation

In order to establish notation, and lay some basic ground work for the development which follows, the essential features

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of modal synthesis are briefly summarized. The equation of motion for each substructure may be written

$$\mu^i \ddot{x}^i + \kappa^i x^i = f_x^{\ i} \tag{1}$$

where μ^i and κ^i denote the mass and stiffness matrices of the ith substructure corresponding to the vector of coordinate displacements x^i, and $f_x^{\ i}$ is a vector of external forces acting on the substructure. This equation may be transformed to a component mode coordinate space by a square matrix of column vectors each representing either a normal (dynamic) mode of the substructure with interface points fixed, or a static mode defining motion over part of the interface boundary. The chief purpose of the modal transformation, however, is to allow a reduction of the coordinate space by truncation of higher order component modes. Thus, if ϕ^{oi} represents a rectangular matrix including all of the static modes and all of the dynamic modes up to a specified frequency, then an *approximate modal transformation* is given by

$$x^i = \phi^{oi} p^{oi} \tag{2}$$

and the original equation of motion may be written

$$m^{ooi} \ddot{p}^{oi} + k^{oo} p^{oi} = f_p^{\ oi} \tag{3}$$

Similar equations may be written for each substructure and arranged in block diagonal form to represent the equations of motion for the complete structural assembly. These may be written

$$m^{oo} \ddot{p}^o + k^{oo} p^o = f_p^{\ o} \tag{4}$$

where, for example,

$$p^o = \begin{Bmatrix} p^{o1} \\ p^{o2} \\ \vdots \\ p^{on} \end{Bmatrix} \quad \text{and} \quad m^{oo} = \begin{bmatrix} m^{oo1} & & & \\ & m^{oo2} & & \\ & & \ddots & \\ & & & m^{oon} \end{bmatrix}$$

These equations are coupled only implicitly through interactive forces included in the vector $f_p^{\ o}$. The final step is to introduce a *compatibility transformation*

$$p^o = \beta q^o \tag{5}$$

whereby the equations of motion are coupled explicitly on the left-hand side and interactive forces cancel on the right-hand side. The final form of these equations may then be written

$$M^{oo} \ddot{q}^o + K^{oo} q^o = f_q^{\ o} \tag{6}$$

and solution of the eigenproblem formed from the homogeneous equations represents an initial approximation to the eigenvalues and eigenvectors of the system.

In subsequent paragraphs, the consideration of additional component modes will require component mode transformations of the form

$$x^i = [\phi^{oi} \vdots \phi^{ni}] p^i \tag{7}$$

where the rectangular matrix ϕ^{ni} represents a set of new component modes added to those, ϕ^{oi}, which were originally chosen. In this case the coupled equations of motion written in terms of component mode coordinates are

$$\begin{bmatrix} M^{oo} & M^{on} \\ M^{no} & M^{nn} \end{bmatrix} \begin{Bmatrix} \ddot{q}^o \\ \ddot{q}^n \end{Bmatrix} + \begin{bmatrix} K^{oo} & K^{on} \\ K^{no} & K^{nn} \end{bmatrix} \begin{Bmatrix} q^o \\ q^n \end{Bmatrix} = \begin{Bmatrix} f_q^{\ o} \\ f_q^{\ n} \end{Bmatrix} \tag{8}$$

Rayleigh Quotient in an Expanded Coordinate Space

Criteria for evaluating convergence of the initial solution, and an algorithm for improving the nonconvergent modes are derived on the basis of Rayleigh quotient minimization in an expanded coordinate space. This space is spanned by the initial selection of modal vectors and the set of newly added ones. A position vector in this space has been denoted by the vector

$$q = \begin{Bmatrix} q^o \\ q^n \end{Bmatrix} \tag{9}$$

where q^o refers to the old modes and q^n to the new. The Rayleigh quotient in this expanded space is denoted by

$$R(q) = \frac{q^T K q}{q^T M q} \tag{10a}$$

where

$$K = \begin{bmatrix} K^{oo} & 0 \\ 0 & K^{nn} \end{bmatrix} \tag{10b}$$

$$M = \begin{bmatrix} M^{oo} & M^{on} \\ M^{no} & M^{nn} \end{bmatrix} \tag{10c}$$

The off-diagonal submatrices of K are null whenever fixed-interface substructure modes are used as discussed by Hurty.[2,8] Consistent with this notation, the initial eigenproblem may be written

$$(K^{oo} - \Lambda_{o_j} M^{oo}) \Phi_{o_j}^{\ o} = 0 \tag{11}$$

where Λ_{o_j} and $\Phi_{o_j}^{\ o}$ denote the initial approximation of the jth system eigenvalue and eigenvector, respectively.

It will be advantageous to make the transformation of coordinates

$$q = \begin{Bmatrix} q^o \\ q^n \end{Bmatrix} = \begin{bmatrix} \Phi_o^{\ o} & 0 \\ 0 & I \end{bmatrix} \begin{Bmatrix} \eta^o \\ \eta^n \end{Bmatrix} = \Phi_o \eta \tag{12}$$

where $\Phi_o^{\ o}$ is a square matrix whose columns are $\Phi_{o_j}^{\ o}$ and I is an identity matrix. The Rayleigh quotient may then be written in terms of the mixed coordinate vector, η, which is seen to include system as well as component displacement coordinates

$$R^*(\eta) = \frac{\eta^T K^* \eta}{\eta^T M^* \eta} \tag{13a}$$

With eigenvectors normalized to give unit modal mass

$$K^* = \begin{bmatrix} \Lambda_o & 0 \\ 0 & \lambda^n \end{bmatrix} \tag{13b}$$

$$M^* = \begin{bmatrix} I & \Phi_o^{\ oT} M^{on} \\ M^{no} \Phi_o^{\ o} & I \end{bmatrix} \tag{13c}$$

where Λ_o is a diagonal matrix of eigenvalues corresponding to Eq. (11) and λ^n represents the set of component eigenvalues associated with the newly added component modes. A convenient feature of the η coordinate system is that the search for the jth eigenvalue will usually begin with the position vector e_j, where e_j denotes the jth column of an identity matrix having the dimensions of the expanded space. In the q coordinate system, the initial value of q_j is

$$q_j = \Phi_o e_j = \begin{Bmatrix} \Phi_{o_j}^{\ o} \\ 0 \end{Bmatrix} \tag{14}$$

A Scaling Transformation

Scaling transformations are frequently used in numerical analysis to adjust the variables to approximately the same order of magnitude. Improvements in accuracy and computational efficiency are thereby realized. The type of scaling transformation considered here is a diagonal matrix whose elements scale the individual degrees of freedom in the displacement vector. Recent investigations of scaling applied to the direct minimization of energy functions have produced encouraging results. Fox and Stanton[10] introduced the idea to solve linear plate bending problems by minimizing the total potential energy. Both the variable metric and the Conjugate Gradient algorithms were used, with and without scaling. Scaling reduced the number of cycles required to converge by as much as an order of magnitude. They used a scaling matrix whose elements were the reciprocal square roots of the diagonal elements of the stiffness matrix. Stanton and Schmit[11] followed the same procedure in solving the nonlinear equilibrium equations for elasto-plastic plates. More recently, Stanton and McGovern[12] showed that a scaling transformation is beneficial in solving the vibration eigenproblem by minimization of the Rayleigh quotient. Results comparable to those of Fox and Stanton were reported.

In the linear statics problem, the stiffness matrix is the Hessian

matrix of the potential energy function. To derive an appropriate scaling matrix for the vibration eigenproblem, Stanton and McGovern used the Hessian matrix, H, of the Rayleigh quotient. Since this matrix is not necessarily positive definite, the elements of the scaling matrix D were defined to be

$$D_{ij} = \frac{\delta_{ij}}{c|H_{ij}|^{1/2}} \tag{15}$$

where $H = \nabla_\eta{}^2 R^*$, δ_{ij} is the Kronecker delta and c is some positive constant.

When the jth mode Φ_{o_j} is nearly convergent, a scaling transformation

$$\eta = D\gamma \tag{16a}$$

is suggested where

$$D = \begin{bmatrix} D^o & \vdots & 0 \\ \cdots & \ddots & \cdots \\ 0 & \vdots & D^n \end{bmatrix} \tag{16b}$$

and the elements of D^o and D^n are

$$D_{ii}{}^o = \begin{cases} 1/(4\Lambda_{o_j}|\Lambda_{o_i} - \Lambda_{o_j}|)^{1/2} : i \neq j \\ 0 \qquad\qquad\qquad\quad : i = j \end{cases} \tag{16c}$$

$$D_{ii}{}^n = 1/(4\Lambda_{o_j}|\lambda_i{}^n - \Lambda_{o_j}|)^{1/2} \tag{16d}$$

It has been found convenient to let the constant $c = (4\Lambda_{o_j})^{1/2}$. The reason for defining $D_{jj}{}^o \equiv 0$ will become apparent when normalization of the eigenvectors is discussed. The Rayleigh quotient expressed in terms of the γ coordinate system will be written

$$\tilde{R}^*(\gamma) = \gamma^T \tilde{K}^* \gamma / \gamma^T \tilde{M}^* \gamma \tag{17}$$

where $\tilde{K}^* = DK^*D$ and $\tilde{M}^* = DM^*D$.

Projection onto an Orthogonal Subspace

The problem of minimizing the Rayleigh quotient to obtain the jth eigenvalue and eigenvector may be stated as follows: find γ such that $\tilde{R}^*(\gamma)$ is a minimum subject to the constraints

$$\eta^T e_k = \gamma^T D\, e_k = 1 \tag{18}$$

and

$$\Phi_\eta{}^{LT} M^* \eta = N^T D\gamma = 0 \tag{19a}$$

where

$$\Phi_\eta{}^L = [\Phi_{\eta_1} \vdots \Phi_{\eta_2} \vdots \cdots \vdots \Phi_{\eta_{j-1}}] \tag{19b}$$

Equation (18) is the expression of a normalization condition on γ while Eq. (19) is the orthogonality constraint. The rectangular matrix N is introduced for notational convenience.

Fox and Kapoor[13,14] approached the solution of this problem (without scaling) by projecting the position and gradient vectors onto a subspace of R reflecting these constraints. In so doing, they were able to minimize R over a restricted domain to determine higher order eigenvalues and eigenvectors. Stanton and McGovern[12] used this method along with a scaling transformation to accelerate convergence. However, the scaling transformation they used did not take into account the orthogonality constraint, nor did the projection matrix incorporate the scaling transformation. As an apparent result, some trouble was reported in searching the restricted space for higher order eigenvalues and eigenvectors. They recommended introducing the orthogonality constraint into the scaling transformation for each higher order mode, but the reverse procedure of incorporating the scaling transformation in the projection matrix is also valid. Indications are that the latter alternative may be preferred for computing the lower order eigenvalues and eigenvectors since it avoids the need to operate on $\tilde{K}^*$ and $\tilde{M}^*$ with the projection matrix which has the dimensions of the expanded space. The disadvantage is that the *projection* of a vector requires more computation because a different matrix of order $(j-1)$ by $(j-1)$ must be inverted for each new jth eigenvalue, whereas Fox and Kapoor were able to use a recursive formula. When j is small, this is of little concern so that the latter alternative appears more favorable.

An arbitrary vector γ may be projected onto a subspace of R by a transformation such as

$$\gamma_p = P\gamma \tag{20}$$

If γ_p is to satisfy Eq. (19a), then it may be expressed in the form

$$\gamma_p = \gamma - DN\alpha \tag{21}$$

where α is a vector of $j-1$ coefficients, as yet unknown. Then α may be determined by premultiplying Eq. (21) by N^TD and using Eq. (19a), giving

$$\alpha = (N^T D^2 N)^{-1} N^T D\gamma \tag{22}$$

Substitution of this result back into Eq. (21) gives

$$\gamma_p = [I - DN(N^T D^2 N)^{-1} N^T D]\gamma \tag{23}$$

Comparison with Eq. (20) suggests that P may be chosen as

$$P = [I - DN(N^T D^2 N)^{-1} N^T D] \tag{24}$$

It is now observed that when the starting vector $\eta_j = e_j$ is used, that having set $D_{jj}{}^o = 0$ in Eq. (16c) insures that the jth element of η_{p_j} will remain equal to unity, since

$$\eta_{p_j} = D\gamma_{p_j} = [I - D^2 N(N^T D^2 N)^{-1} N^T]\eta_j \tag{25}$$

A projection matrix for the gradient vector may be derived in somewhat the same way. A Lagrange function for the constrained minimization problem [Eqs. (17–19)] is first defined as

$$L(\gamma) = \tilde{R}^*(\gamma) - \gamma^T DN\alpha - (\gamma^T D\, e_k - 1)\alpha_k \tag{26}$$

where in this case α is a vector of Lagrange multipliers and α_k is a scalar multiplier. Minimization of the function $L(\gamma)$ thus transforms the constrained minimization problem to one which is unconstrained. A necessary condition for L to be a minimum is given by the Euler-Lagrange equations which are

$$\nabla L = \nabla \tilde{R}^* - DN\alpha - De_k\alpha_k = 0 \tag{27}$$

Solving first for α and then α_k and substituting their values into Eq. (27) leads to the result

$$g_p = \nabla_\gamma L(\gamma) = P' P \nabla_\gamma \tilde{R}^*(\gamma) = P' P g \tag{28}$$

where

$$P' = [I - PDe_k(e_k{}^T DPDe_k)^{-1} e_k{}^T D] \tag{29}$$

The symbol g and g_p denote the gradient and projected gradient vectors in the scaled coordinate space. For the present application this result may be simplified considerably. Since a constant scaling matrix is to be used and the search for the jth mode will always begin with $\eta_j = e_j$, the term $(e_j{}^T DPDe_j)^{-1}$ is undefined. However, one may define

$$De_j(e_j{}^T DPDe_j)^{-1} e_j{}^T D \equiv \frac{1}{P_{jj}} e_j e_j{}^T = e_j e_j{}^T \tag{30}$$

which is consistent with the way in which D was defined. This result guarantees that a step $\delta\gamma$ taken in the direction of steepest descent will have no component in the direction of e_j.

That is

$$P' = (I - e_j e_j{}^T) \tag{31}$$

From this result one may go on to conclude that the presence of P' is in fact redundant since the jth element of g is already zero by virtue of the scaling matrix D. It therefore follows that

$$g_p = (I - e_j e_j{}^T)Pg = Pg \tag{32}$$

With Eqs. (20, 24, and 32) the vector γ and the gradient vector g may be projected onto a scaled subspace which is orthogonal to the lower order eigenvectors. When it happens that all of the lower order eigenvectors, $\Phi_i (i < j)$, are convergent in the first approximation so that $\Phi_{\eta_i} \approx e_i$ $(i < j)$, it follows from $\eta_j = D\gamma_j = e_j$, that

$$N^T D\gamma_j = N^T e_j = \Phi_\eta{}^{LT} M^* e_j = 0 \tag{33}$$

since

$$\Phi_{\eta_i}{}^T M^* e_j = e_i{}^T M^* e_j = 0, \quad i < j \tag{34}$$

Therefore, according to Eq. (23), even though $P \neq I$, one finds that

$$\gamma_{p_j} = \gamma_j \tag{35}$$

Under the same conditions, a similar conclusion is reached[15] for g, so that

$$g_{p_j} = g_j \tag{36}$$

Convergence Indicators

The Rayleigh quotient when scaled and projected onto a subspace orthogonal to the lower order modes may be written

$$\tilde{R}^*(\gamma_p) = \gamma_p{}^T\tilde{K}^*\gamma_p/\gamma_p{}^T\tilde{M}^*\gamma_p \tag{37}$$

The more powerful minimization algorithms rely on the gradient of this function to help direct the search. In order to restrict the search to the proper subspace, the gradient vector must also be orthogonal to the lower order modes. The projected gradient vector corresponding to the position vector γ_p is written

$$g_p = 2P[\tilde{K}^* - \tilde{R}^*(\gamma_p)\tilde{M}^*]/\gamma_p{}^T\tilde{M}^*\gamma_p \tag{38}$$

A small step h_p in the direction of steepest descent $s_p = -g_p$ will tend to make $\tilde{R}^*(\gamma_p)$ smaller. That is, for $\delta\gamma_p = h_p s_p$

$$\tilde{R}^*(\gamma_p + \delta\gamma_p) < \tilde{R}^*(\gamma_p) \tag{39}$$

An optimum step h_p' in this direction provides an optimum lower bound on the eigenvalue error $|\delta\Lambda_j|$ since

$$|\delta\Lambda_j| \geqq |\delta\tilde{R}^*(\gamma_p)| = |\tilde{R}^*(\gamma_p) - \tilde{R}^*(\gamma_p + \delta\gamma_p)| \tag{40}$$

Bradbury and Fletcher[16] have shown in effect that the condition

$$\partial\tilde{R}^*(\gamma_p + h_p s_p)/\partial h_p = 0 \tag{41}$$

leads to a quadratic equation

$$ah_p{}^2 + bh_p + c = 0 \tag{42}$$

In this case

$$a = (s_p{}^T\tilde{K}^*s_p)(\gamma_p{}^T\tilde{M}^*s_p) - (\gamma_p{}^T\tilde{K}^*s_p)(s_p{}^T\tilde{M}^*s_p) \tag{43a}$$

$$b = (s_p{}^T\tilde{K}^*s_p)(\gamma_p{}^T\tilde{M}^*\gamma_p) - (\gamma_p{}^T\tilde{K}^*\gamma_p)(s_p{}^T\tilde{M}^*s_p) \tag{43b}$$

$$c = (\gamma_p{}^T\tilde{K}^*s_p)(\gamma_p{}^T\tilde{M}^*\gamma_p) - (\gamma_p{}^T\tilde{K}^*\gamma_p)(\gamma_p{}^T\tilde{M}^*s_p) \tag{43c}$$

Two values of h_p satisfy Eq. (42). Since $\tilde{R}^*$ is bounded, one value must correspond to a minimum of $R^*(\gamma_p + h_p s_p)$ along s_p while the other corresponds to a maximum. The minimum value is designated h_p'. Correspondingly

$$\delta'\gamma_p = h_p's_p \tag{44}$$

$$\delta'\tilde{R}^*(\gamma_p) = \tilde{R}^*(\gamma_p) - \tilde{R}^*(\gamma_p - \delta'\gamma_p) \tag{45}$$

The quantity $\delta'\tilde{R}^*(\gamma_p)$ provides a measure of eigenvalue error while $\delta'\gamma_p$ provides a corresponding measure of eigenvector error. The gradient vectors (either projected or unprojected) provide additional indicators of convergence since $g_p = g = 0$, whenever the position vector γ is a true eigenvector.

Some insight into the meaning of these quantities is gained by considering the case where truncation errors are small, that is

$$|\delta\Lambda_j| = |\Lambda_j - \Lambda_{o_j}| \ll \Lambda_j \tag{46a}$$

$$|\delta\Phi_j| = |\Phi_j - \Phi_{o_j}| \ll |\Phi_j| \tag{46b}$$

Linear perturbation analysis[5,15] shows that to first-order approximation

$$\delta\Lambda_j = -\Lambda_{o_j}{}^2\Phi_{o_j}{}^oM^{on}(\lambda^n - \Lambda_{o_j}I)^{-1}M^{no}\Phi_{o_j}{}^o \tag{47}$$

and

$$\delta\Phi_j = \begin{Bmatrix} \delta\Phi_j{}^o \\ \cdots \\ \delta\Phi_j{}^n \end{Bmatrix} \tag{48a}$$

where

$$\delta\Phi_j{}^o = 0 \tag{48b}$$

$$\delta\Phi_j{}^n = \Lambda_{o_j}(\lambda^n - \Lambda_{o_j}I)^{-1}M^{no}\Phi_{o_j}{}^o \tag{48c}$$

As Hurty[5] points out, Eq. (47) may be simplified by partitioning $\Phi_{o_j}{}^o$ into two subvectors

$$\Phi_{o_j}{}^o = \begin{Bmatrix} \Phi_{o_j}{}^B \\ \cdots \\ \Phi_{o_j}{}^N \end{Bmatrix} \tag{49}$$

corresponding to the *boundary* (static) mode coordinates and *normal* (dynamic) mode coordinates. Orthogonality of the dynamic modes dictates that

$$M^{no} = [M^{nB} \vdots M^{nN}] = [M^{nB} \vdots 0] \tag{50}$$

so that

$$M^{no}\Phi_{o_j}{}^o = M^{nB}\Phi_{o_j}{}^B \tag{51}$$

Under similar conditions, it has been shown[15] after a somewhat lengthy derivation that Eqs. (45) and (44) reduce to Eqs. (47) and (48), respectively. This is equivalent to stating that $\tilde{R}^*(\gamma_p)$ is minimized to first-order approximation by taking a single step in the direction of the steepest descent vector $s_p = -g_p$. What is implied here is that the better the initial solution is, the more accurately the scaling transformation will point s_p in the direction of the minimum. A closer look at this vector is warranted.

The gradient of R^* evaluated at a point in the unscaled coordinate space determined by the initial eigenvector approximation Φ_{o_j} is

$$\nabla_\eta R^*(e_j) = \frac{2[K^* - R^*(e_j)M^*]e_j}{e_j{}^TM^*e_j} \tag{52}$$

Expanding these quantities gives

$$\begin{aligned} \nabla_\eta R^*(e_j) &= 2\left(\begin{bmatrix} \Lambda_o & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & \lambda^n \end{bmatrix} - \Lambda_{o_j}\begin{bmatrix} I & \vdots & \Phi_o{}^{oT}M^{on} \\ \cdots & \cdots & \cdots \\ M^{no}\Phi_o{}^o & \vdots & I \end{bmatrix}\right)e_j \\ &= 2\begin{Bmatrix} 0 \\ \cdots \\ -\Lambda_{o_j}M^{no}\Phi_{o_j}{}^o \end{Bmatrix} \end{aligned} \tag{53}$$

From this it is clear that $\nabla_\eta R^*(e_j)$ is orthogonal to the original coordinate space. It is further noted that

$$\{\nabla_\eta R^*(e_j)\}^T\{\nabla_\eta R^*(e_j)\} = 4\Lambda_{o_j}{}^2\Phi_{o_j}{}^oM^{on}M^{no}\Phi_{o_j}{}^o \tag{54}$$

which is similar in form to Eq. (47). In the scaled coordinate space it is found that

$$g = \nabla_\gamma\tilde{R}^*(\gamma) = D\nabla_\eta R^*(e_j) \tag{55}$$

so that

$$\begin{aligned} g^Tg = 4\Lambda_{o_j}{}^2\Phi_{o_j}{}^{oT}M^{on}D^2M^{no}\Phi_{o_j}{}^o = \\ -\Lambda_{o_j}\Phi_{o_j}{}^{oT}M^{on}(\lambda^n - \Lambda_{o_j}I)^{-1}M^{no}\Phi_{o_j}{}^o \end{aligned} \tag{56}$$

which is identically equal to $\delta\Lambda_j/\Lambda_{o_j}$ from Eq. (47). Thus it is seen that $g^Tg = |g|^2$ provides an alternate interpretation of Eq. (47). The significance of this result is that no small error assumptions were made in deriving Eq. (56). Whenever these assumptions break down, the right-hand side of Eq. (56) may no longer be interpreted as a first-order approximation of the eigenvalue error. It may still be interpreted as the squared magnitude of the scaled gradient vector, however. Whenever the small error assumptions do hold, it has already been pointed out that $g_p = g$. That is, the projection matrix has no effect on g to first-order approximation.

The eigenvector error indicator given by Eq. (48) has a useful physical interpretation. Again it is emphasized that Eq. (48) is valid only when truncation errors are small. To first-order approximation, the eigenvector error corresponding to the original component mode coordinates is zero. This is consistent with the fact that the gradient vector is initially orthogonal to the original coordinate space. Elements of the error vector $\delta\Phi_j{}^n$ are of the following form:

$$\delta\Phi_{ij}{}^n = \frac{F_{ij}}{Z_{ij}} \tag{57}$$

where

$$F_{ij} = \Lambda_{o_j}\sum_k M_{ik}{}^{nB}\Phi_{o_{kj}}{}^B \tag{58}$$

is the generalized constraint force acting in coordinate i, equal and opposite in direction to the residual force or force unbalance resulting from harmonic motion in mode Φ_{o_j}. The denominator

$$Z_{ij} = (\lambda_i{}^n - \Lambda_{o_j}) \tag{59}$$

is the dynamic impedance offered by the system tending to resist that force. When the impedance is high as a result of large frequency separation, the displacement of the structure is not affected appreciably. The quantity $M_{ik}{}^{nB}$ is of the form

$$M_{ik}{}^{nB} = \phi_i{}^{nT}\mu\phi_k{}^B \tag{60}$$

where μ represents the discrete coordinate mass matrix of a particular substructure and $\phi_k{}^B$ and $\phi_i{}^n$ represent a static and a

dynamic mode of that substructure. Then $M_{ik}{}^{nB}$ may be interpreted as the constraint force applied in coordinate i which is required to react a distributed inertia load of $\mu\phi_i{}^B\ddot{q}_k{}^B$ when $\ddot{q}_k{}^B = -1$. To determine the generalized constraint force F_{ij},

$$\ddot{q}_k{}^B = -\Lambda_{o_j}\Phi_{o_{kj}}{}^B \tag{61}$$

so that the total load distribution is the sum

$$-\sum_k \Lambda_{o_j}\mu\phi_k{}^B\Phi_{o_{kj}}{}^B \tag{62}$$

of contributions from each of the k boundary coordinates. When this distributed load is multiplied by the displacement function of the ith coordinate, and the resultant product is integrated over the substructure, the result is

$$-F_{ij} = -\phi_i{}^{nT}\sum_k \Lambda_{o_j}\mu\phi_k{}^B\Phi_{o_{kj}}{}^B \tag{63}$$

which is equivalent to Eq. (58). The truncation of component mode coordinates is equivalent to constraining the motion of the structure in the sense that no motion is permitted in the direction of the coordinates not included. The constraint forces F_{ij} are the forces required to implement these constraints.

The form of Eq. (48) in conjunction with this physical interpretation seems to suggest that the component displacement functions ϕ and their relationship to the system eigenvectors Φ may have a stronger influence on convergence than do the corresponding eigenvalues λ and Λ. This conclusion is consistent with experience which indicates that system modes obtained by modal synthesis are usually found to be convergent through system frequencies including 50%–70% of the range spanned by the uncoupled component frequencies. If the frequency relationship (or impedance) governed convergence, one would expect convergence over a much smaller range.

Minimization of the Rayleigh Quotient

While criteria for assessing convergence have received considerable attention in recent years, relatively little attention has been devoted to the problem of improving nonconvergent modes after an initial solution is obtained. Bajan, Feng, and Jaszlics[9] have described a procedure requiring several eigenproblem solutions of the same size as the initial one. A transformation method such as Householder's method is used each time so that all of the modes are solved for repeatedly. This can be particularly inefficient when only a few modes require improvement. By contrast, the minimization approach is an iterative one operating on only one mode at a time; the convergent ones may be skipped. The initial solution provides information useful in transforming the succeeding problem to a form which allows the minimization process to converge rapidly.

Various methods for minimizing a function of several variables are available. These include both gradient and nongradient methods. In general, gradient methods are more powerful since they utilize more information about the function. The classical method of this type is the method of steepest descents, so named because each direction of search corresponds to that of the negative gradient vector which always points "downhill." Although popular at one time, experience has shown the method to converge slowly if the function has any appreciable eccentricity.

More attractive methods have the property of quadratic convergence, in that for a quadratic function of n variables, the process will converge in at most n steps, apart from roundoff error. Straeter and Hogge[17] have made a comparison of several gradient dependent minimization techniques having the property of quadratic convergence. Two of these, the method of Davidon[18] as amended by Fletcher and Powell[19] and the method of Conjugate Gradients adapted by Fletcher and Reeves[20] from some earlier work of Hestines and Stiefel,[21] reduce an n-dimensional unconstrained minimization to a sequence of one-dimensional minimizations. Using Rosenbrock's parabolic valley function as a basis for comparing the methods, Straeter and Hogge concluded that the Fletcher-Powell method showed a faster rate of convergence.

Bradbury and Fletcher,[16] on the other hand, have compared the two methods for minimizing the Rayleigh quotient of a general eigensystem. In this case they showed that the one-dimensional minimization problem may be solved in closed form. The Conjugate Gradient and Fletcher-Powell methods for computing the smallest eigenvalues of random matrices (random elements between ± 100) up to order 70 were compared on the basis of execution time. The Fletcher-Powell method took $1\frac{1}{2}$ to 2 times longer than the Conjugate Gradient method even though fewer iterations were actually required.

Other considerations which relate to the special case at hand make the Conjugate Gradient method even more attractive. In the first place, the Fletcher-Powell method requires the storage and manipulation of a full n by n matrix at each step of the search. This alone practically disqualifies it for the present application since one of the main objectives is to improve convergence without having to fit a larger matrix in core. The sparsity of the mass and stiffness matrices which result from the modal synthesis formulation may be used to advantage in computing the Rayleigh quotient and its gradient so that the storage of a full n by n matrix is not required by the Conjugate Gradient method.

Secondly, the Fletcher-Powell method derives its principal advantage from its ability to generate better search directions. The auxiliary n by n matrix is used in a sense to approximate the local curvature of the function in order to adjust the metric of the space for more rapid convergence. The procedure is very general. Again, with the present formulation, it has been shown that the Hessian matrix *corresponding to a good starting vector* is nearly diagonal so that a good approximation of the curvature in the region of a lower order eigenvector is provided by just the diagonal of the matrix. Furthermore, the diagonal elements are nearly constant for small changes in the eigenvector. The diagonal matrix can then be used to define a constant scaling transformation which, in conjunction with the Conjugate Gradient method, should produce search directions on a par with those generated by the Fletcher-Powell method, at considerably less expense. Thus, for the present application the Conjugate Gradient method with scaling appears to combine the advantages of both methods.

The Conjugate Gradient algorithm for minimizing the Rayleigh quotient in the proper subspace may be written[15,20]

$$\gamma_p{}^o = P\gamma^o;\ \gamma^o = \text{arbitrary} \tag{64a}$$

$$g_p{}^o = P\nabla_\gamma \tilde{R}^*(\gamma_p{}^o) \tag{64b}$$

$$s_p{}^o = -g_p{}^o \tag{64c}$$

$$\gamma_p{}^{i+1} = \gamma_p{}^i + h_p{}^i s_p{}^i \tag{64d}$$

$$g_p{}^{i+1} = P\nabla_\gamma \tilde{R}^*(\gamma_p{}^{i+1}) \tag{64e}$$

$$\beta_p{}^i = |g_p{}^{i+1}|^2/|g_p{}^i|^2 \tag{64f}$$

$$s_p{}^{i+1} = -g_p{}^{i+1} + \beta_p{}^i s_p{}^i \tag{64g}$$

In this case the Rayleigh quotient of the projected vector γ_p (dropping the superscript i) is given by

$$\tilde{R}^*(\gamma_p) = \frac{\gamma_p{}^T\tilde{K}^*\gamma_p}{\gamma_p{}^T\tilde{M}^*\gamma_p} = \frac{\gamma_p{}^T DK^* D\gamma_p}{\gamma_p{}^T DM^* D\gamma_p} \tag{65}$$

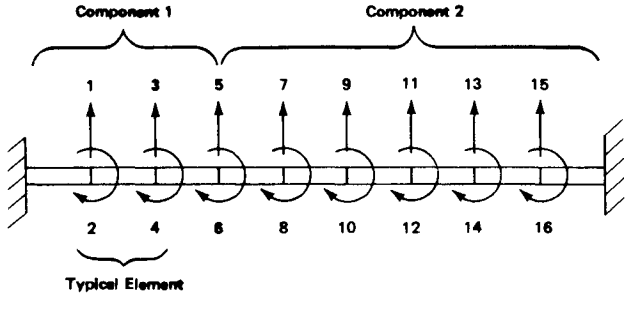

Fig. 1 Finite element model of a 16-dof fixed-fixed beam.

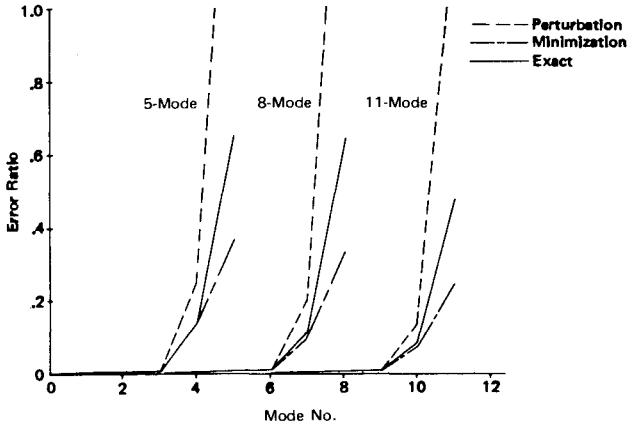

Fig. 2 Eigenvalue error in modal synthesis of a 16-dof structure.

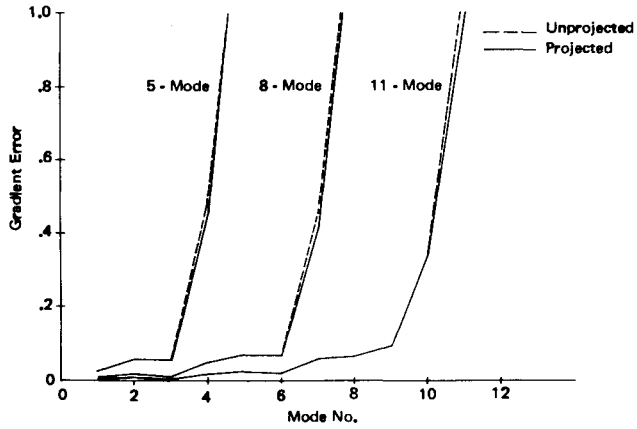

Fig. 4 Gradient error in modal synthesis of a 16-dof structure.

where

$$D\gamma_p = DP\gamma = D[I - DN(N^TD^2N)^{-1}N^TD]\gamma = [I - D^{2N}(N^TD^2N)^{-1}N^T]D\gamma \tag{66}$$

and $D\gamma = \eta$. Similarly

$$g_p = P\nabla_\gamma \tilde{R}^*(\gamma_p) = \frac{2PD[(K^* - \tilde{R}^*(\gamma_p)M^*]D\gamma_p}{\gamma_p{}^TDM^*D\gamma_p} \tag{67}$$

From a computational standpoint, one would store the vector $D\gamma_p{}^i = \eta_p{}^i$ rather than $\gamma_p{}^i$ itself. In fact, $\gamma_p{}^i$ alone is not completely defined due to the singularity of D. Again, $N^TD\gamma^o = 0$ implies that $\gamma_p{}^o = \gamma^o$

Example Problem

The present example is a beam with both ends clamped, modeled as a two-component structure. The beam is subdivided into nine identical elements. The first three comprise Component 1, while the remaining six comprise Component 2. The complete structure has a total of 16 degrees of freedom, as shown in Fig. 1. Two of these are associated with the common interface boundary of the components. Of the remaining 14 degrees of freedom, four are considered to be internal coordinates of Component 1 and ten of Component 2. Full mass matrices are utilized, consistent with the static deformation shapes of the basic element.

Coordinate reduction is accomplished by first computing the fixed-interface modes of the two components. Four modes are obtained for Component 1 and ten for Component 2. Reduced sets of equations based on 5, 8, and 11 degrees of freedom are obtained by transformation to distributed coordinates including the two static modes and combinations of (1, 2), (2, 4), and (3, 6) of the lowest modes of Components 1 and 2, respectively.

Three types of error indicators are considered. Eigenvalue error ratios are of the form $-\delta\Lambda_j/\Lambda_{o_j}$, as given by Eq. (47). Eigenvector errors are presented in a similar form, $|\delta\Phi_j|/|\Phi_{o_j}|$, as given by Eq. (48). A key element of the eigenvector is held constant in this case. There are many ways to measure eigenvector error; the present method provides a useful measure of the over-all error for the given problem, and has been chosen for the purpose of illustration. Gradient error magnitudes of the form $|g|$ and $|g_p|$ are also compared. As mentioned earlier

$$|g|^2 \approx -\delta\Lambda_j/\Lambda_{o_j} \tag{68}$$

when modal errors are small.

A comparison of eigenvalue error indicators for the three cases is shown in Fig. 2. Both the perturbation error and the minimization error are indistinguishable from the exact error in all but the last two modes of the original approximation for each case.

A comparison of eigenvector error indicators is shown in Fig. 3. Again, the perturbation and minimization error estimates closely resemble the exact error for the nearly convergent modes. The minimization error appears to be a lower bound on eigenvector as well as eigenvalue error in these examples, although it is not generally true.

Figure 4 presents a comparison of the projected and unprojected gradient magnitudes. These two quantities appear to remain close even when the lower modes are not all convergent. Similar results have been obtained for other problems.

To give an indication of how the minimization procedure converges during the modal improvement phase of the analysis,

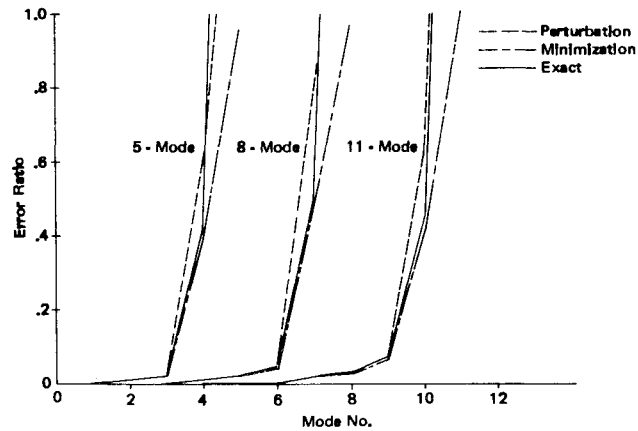

Fig. 3 Eigenvector error in modal synthesis of a 16-dof structure.

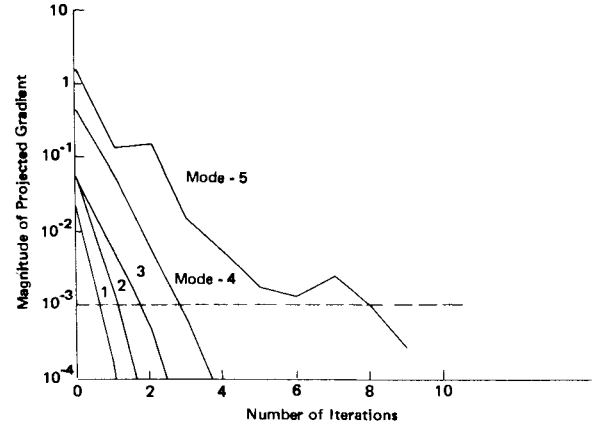

Fig. 5 Convergence of modes initially obtained from five-mode synthesis of a 16-dof structure.

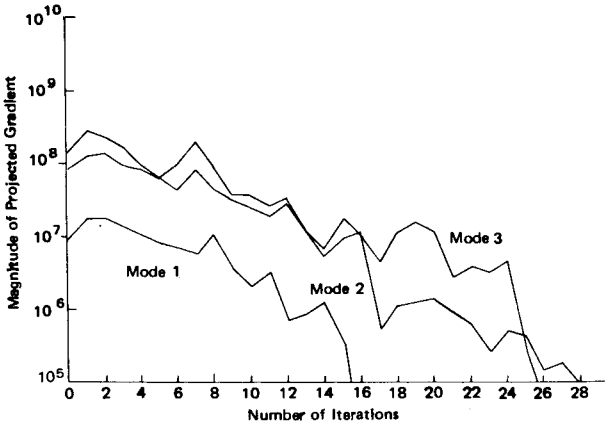

Fig. 6 Convergence of modes initially obtained from five-mode synthesis of a 16-dof structure, unscaled coordinate system.

values of $|g_p|$ are plotted in Fig. 5 as functions of the number of steps taken. A value of $|g_p| = 0.001$ corresponds approximately to six-digit accuracy in the eigenvalue. Convergence of the first three modes to four-digit accuracy ($|g_p| = 0.01$) is achieved in only one step. The constant scaling transformation in this case is very poor for the fifth mode. The minimization still converges, but more slowly. The advantage of scaling is illustrated by Fig. 6, in which the magnitude of the unscaled projected gradient is plotted. In this case, six-digit accuracy was achieved in the eigenvalues when this number reached 10 (Ref. 5). A somewhat larger problem yielded similar results. A 51 degree of freedom structure consisting of three components, for which the initial solution included only nine of the substructure modes, exhibited the convergence characteristics shown in Fig. 7 when the modal vector space was expanded to include 27 of the 51 modes. This example shows that the rate of convergence does-not dpend on the number of degrees of freedom which, in this case, is 27.

Conclusions

A number of convergence indicators have been derived. The perturbation approach adopted by Hurty for estimating eigenvalue error has been extended to yield a corresponding expression for the eigenvector error. A single step in the minimization of the Rayleigh quotient yields closed-form expressions for the eigenvalue and eigenvector errors which agree with the perturbation results whenever the small error assumptions hold. Beyond that, the perturbation results become invalid while the indicators derived from the minimization approach are still meaningful.

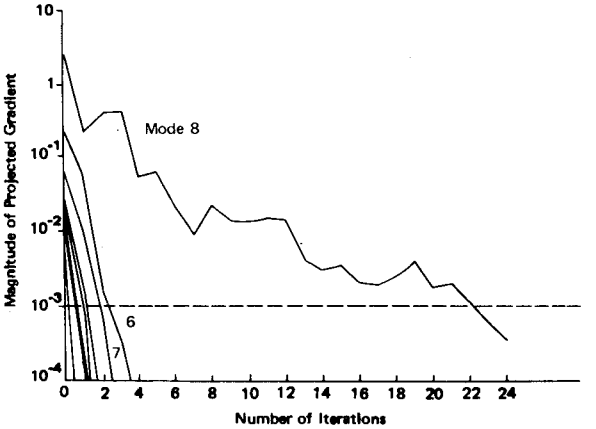

Fig. 7 Convergence of modes initially obtained from nine-mode synthesis of a 51-dof structure.

The gradient of the Rayleigh quotient may be evaluated before and after it is projected onto the subspace orthogonal to the lower modes. As truncation errors become larger, differences do show up, as one would expect. As it turns out, the inner product of the unprojected gradient vector in the scaled coordinate space is identical to Hurty's approximation of the eigenvalue error. The significance of this result is that it offers a different interpretation of Hurty's formula which is meaningful for even large modal errors. This presumably explains why Hurty's formula has been found reliable for judging convergence even when the underlying assumptions break down.

Use of the conjugate gradient algorithm with the appropriate scaling transformation has been found to minimize the Rayleigh quotient in only a few steps. One-step convergence is achievable for modes with small error. The number of steps appears to depend primarily on the magnitude of error and not on the number of degrees of freedom involved. This advantage, combined with the modest storage requirements of the conjugate gradient algorithm, makes the method attractive compared to alternative procedures.

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Shock Wave Boundary-Layer Interactions in Laminar Transonic Flow

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A solution is presented for a shock interacting with an unseparated laminar boundary layer in transonic flow. The method of matched asymptotic expansions is employed. The flowfield is divided into three regions: the transonic flow external to the boundary layer, an outer boundary-layer zone, and a thin viscous sublayer near the wall. The interaction occurs over a region with a length of order $Re^{-3/8}(M_\infty-1)^{-3/8}$ and a height of order $Re^{-3/8}(M_\infty-1)^{-7/8}$ where Re is the Reynolds number based on the boundary-layer length and M_∞ is the freestream Mach number. For the case of an incoming oblique shock, the shock is weakened as it approaches the boundary layer, an expansion fan is formed at the intersection of the shock and the boundary layer, and compression waves formed both upstream and downstream of the interaction coalesce to form the reflected shock. Numerical solutions for the wall pressure and other flow properties and a flow picture of the interaction region are presented for such a case. The results apply when $M_\infty-1$ is between $O(Re^{-7/15})$ [limit when boundary-layer displacement effects dominate shock effects] and $O(Re^{-1/5})$ [boundary-layer separation limit].

Nomenclature

$a = \bar{a}/\bar{a}_\infty{}^*$ = nondimensional speed of sound
E = gage parameter, U-velocity component
$k = \bar{k}/\bar{k}_\infty{}^*$ = nondimensional thermal conductivity coefficient
$\bar{L}$ = distance, leading edge to shock intersection
$\bar{L}_x, \bar{L}_y$ = local characteristic lengths
M = Mach number
$P = \bar{P}/\bar{\rho}_\infty{}^*\bar{a}_\infty{}^{*2}$ = nondimensional pressure
$Pr^* = \bar{C}_p\bar{\mu}_\infty{}^*/\bar{k}_\infty{}^*$ = Prandtl number
$Re^* = \bar{\rho}_\infty{}^*\bar{a}_\infty{}^*\bar{L}/\bar{\mu}_\infty{}^*$ = Reynolds number
$T = \bar{T}/(\bar{a}_\infty{}^{*2}/\bar{C}_p)$ = nondimensional temperature
$U = \bar{U}/\bar{a}_\infty{}^*$; $V = \bar{V}/\bar{a}_\infty{}^*$ = nondimensional velocity components
$X = (\bar{X}-\bar{L})/\bar{L}$; $Y = \bar{Y}/\bar{L}$ = nondimensional coordinates
$x; y$ = stretched coordinates
γ = ratio of specific heats
$\gamma(A, z) = \int_0^z s^{(A-1)}e^{-s}ds$ = incomplete gamma function
$\Gamma(A)$ = gamma function
ε = deviation of flow velocity from sonic
Λ' = shock strength parameter
$\mu = \bar{\mu}/\bar{\mu}_\infty{}^*$ = nondimensional viscosity coefficient
$\rho = \bar{\rho}/\bar{\rho}_\infty{}^*$ = nondimensional density
δ, ν, π, τ = gage parameters

Superscripts
$-$ = dimensional quantity
$*$ = sonic value
$\hat{}$ = inviscid rotational flow region
$+$ = viscous sublayer
$\sim$ = transonic flow region

Subscripts
∞ = incoming flow

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Index categories: Boundary Layers and Convective Heat Transfer—Laminar; Shock Waves and Detonations; Subsonic and Transonic Flow.

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Introduction

IT is well known that a boundary layer greatly modifies the simple shock reflection at a solid surface and the attendant abrupt increase in surface pressure predicted by inviscid theory.[1,2] With a boundary layer included, the structure changes from a point of intersection of a shock and the surface, to a region of interaction between the shock and the boundary layer, and the pressure varies continuously.

In this paper, the interaction region between a shock wave and a boundary layer is studied for the case where the external flow is transonic and the boundary-layer flow is laminar and unseparated from a flat wall. The compelling reason for studying such an interaction problem is the application to transonic