Performance of Eigensolvers in Modal Analyses of Nuclear Plant Building Structures

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SUMMARY

The modal time history analysis of nuclear plant building structures subjected to dynamic excitations requires the computation of free vibration modes and frequencies. The models are extremely complex and are characterized by a large number of equations, a large half-bandwidth and a large number of modes and frequencies to be computed.

Several improved eigensolution routines have been offered on the software market to address this situation. They are determinant search methods, subspace iteration methods with shifting, the Lanczos and the Householder QR-methods.

The large size of the models as well as the large number of modes and frequencies requires a thorough investigation of the performance characteristics of these eigensolution routines before a choice is made of the most suitable one. While their performance with carefully selected benchmark problems may be impressive their application to building models with unexpectedly clustered free vibration characteristics may pose a number of problems. These include lack of convergence, skipping of modes, exceeding demands on secondary storage capacities, exceeding allotted run times and progressive deterioration of accuracy. The most serious problem is the excessive time the free vibration analysis spends being resident in the computer (wall clock time).

In the present paper the computations are carried out with different eigensolution routines on a number of large size nuclear plant structural models. A number of performances characteristics are recorded to offer some basis of comparison for the user of such algorithms.

1. INTRODUCTION

The analysis of nuclear plant building structures to be discussed here aims for the generation of displacement and acceleration response spectra which are to be used in the analysis of internal secondary structures. The most popular approach proceeds through a modal analysis requiring, as an initial step, the determination of the free vibration characteristics of the entire system. In recent years the systems to be analyzed have grown in complexity. The frequency range has been drastically expanded. This has been done in an effort to keep the numerical model close to the realities of the structural configuration and to the loading time histories.

In a modal time history analysis of such a system the main burden of the numerical computation lies with the determination of the free vibration characteristics. Cost and accuracy both play a major role. A number of improved eigensolution routines have been offered on the software market to address this situation.

The present paper explores cost and accuracy of a number of eigensolution routines which have been applied to models of nuclear plant building structures with several thousand degrees of freedom and with several hundred free vibration modes and frequencies to be computed.

2. EIGENSOLUTION METHODS

Four principal eigensolution methods have been applied: determinant search methods; subspace iteration methods without shift, with user-activated shift, and with progressive forward shifting; Lanczos QR-method; Householder QR-method. Cost saving by exploiting model symmetry is considered.

2.1 DETERMINANT SEARCH

The computational procedure of the determinant search method [1] consists of five building blocks; secant iteration and Sturm sequence check; inverse iteration; Gram-Schmid orthogonalization of the last six calculated eigenvectors; Rayleigh quotient shift if convergence is slow; and computation of error bounds. The procedure has been available [2] in the subroutine SECANTD in which the decomposition $\underline{K} = \underline{L} \underline{D} \underline{L}^T$ is carried out by the subroutine BANDET without the use of secondary storage. While this solution algorithm is relatively fast it is limited by the available primary storage capacity. For large systems consisting of several thousand degrees of freedom and a half-bandwidth of several hundred, a secondary storage scheme is mandatory. An efficient scheme is the skyline, column-wise storage of a sparse matrix in blocks. The corresponding solution algorithm is called COLDET. The details of skyline decomposition are explained in [3].

2.2 SUBSPACE ITERATION

The subspace iteration procedure has been available for some time [2]. Its application to large eigenvalue problems, that is, a large number

of requested eigenpairs (ω_j, ϕ_j) of structural models with a large number of equations and a large half-bandwidth exhibits a number of serious drawbacks. If there are m eigenvalues to be computed, conventional subspace iteration transforms to a subspace stiffness and mass matrix (see Tables 1 and 2)

$$\underline{K}^* = \tilde{\underline{X}}^T \underline{K} \tilde{\underline{X}} \quad , \quad \underline{M}^* = \tilde{\underline{X}}^T \underline{M} \tilde{\underline{X}} \quad (1)$$

where $\underline{K}^*$ and $\underline{M}^*$ are symmetric but fully populated. $\underline{K}$ is the system stiffness matrix, $\underline{M}$ is the diagonal system mass matrix and $\tilde{\underline{X}}$ contains the approximation vectors of m trial vectors. The storage requirement for the solution of the transformed eigenvalue problem with $\underline{K}^*$ and $\underline{M}^*$ by the Jacobi method is $2m(m+1)$. When the total available primary storage is limited, the maximum size of the subspace is fixed. With m being very large in addition to a number of equations n and a large half-bandwidth m_k of the system stiffness matrix $\underline{K}$ another storage problem arises with the solution of the linear equations

$$\underline{K} \tilde{\underline{X}} = \underline{Y} \quad . \quad (2)$$

The stiffness matrix $\underline{K}$ and the vectors $\tilde{\underline{X}}$ and $\underline{Y}$ are blocked so that $n_b \cdot n_{eqb} = n$, where n_b is the number of blocks and n_{eqb} is the number of equations in a block. To cut down on the input/output operations during the solution of eq.(2) it is important to make n_{eqb} as large as possible. If the m vectors are not all processed at once the block size can be increased thus expanding slightly the size limitation for the eigensolution procedure.

The most serious drawback of the subspace iteration, however, is the slow convergence when the size of the subspace is large [4]. A given range of frequencies to be explored in a model can be divided into a number of small subspaces when a shift is used. The shifted eigenvalue problem $(\omega_j^2 = \mu + \gamma_j)$

$$\hat{\underline{K}} \underline{\Phi} = \underline{\gamma} \underline{M} \underline{\Phi} \quad , \quad (3)$$

with $\hat{\underline{K}} = \underline{K} - \mu \underline{M}$ (where μ is the shift value) is then solved for a given frequency range, with a known number of frequencies to be determined. The size of the subspace, m , can then be kept at a level where no storage and accuracy problems arise.

User Activated Shift. - A solution procedure in which the user activates the shift (Table 1) allows the large eigensolution problem to be solved at a leisurely pace determined by the available primary storage. By permitting overlap of the frequency ranges analyzed the problems of bad convergence at the upper end of each subspace can be controlled. Also, the shift value can be chosen at a convenient point within the frequency range in order to accelerate the convergence. The results of the individual subspace iteration solutions are merged in the end on one file for use in the subsequent modal solution algorithms.

Progressive Forward Shifting. - An automatic shifting procedure has been developed in Ref.[5]. The solution procedure is shown in Table 2. The subspace is kept at $12 \leq m \leq n^{(1/2)}$. The shifting strategy determines when it

is appropriate to perform a shift based on the number of operations required for an iteration without or with a new shift. The program determines what new shift value should be used. The number of operations is based on the convergence behavior of the current and previous iteration. When i_t iterations are needed before the next eigenvalue converges then a new shift is performed if $n_{\text{opd}} + 2n_{\text{opc}} < i_t n_{\text{opc}}$, where n_{opd} is the number of operations for one matrix decomposition and n_{opc} is the number of operations for one iteration cycle. The new shift value μ is chosen just below a projection of the next unconverged eigenvalue for iteration $k+1$,

$$\lambda_{\text{proj}} = \frac{\lambda_{k-1} - \lambda_{k-2} \lambda_k}{2\lambda_{k-1} - \lambda_{k-2} - \lambda_k} \quad (4)$$

Here lies one of the drawbacks of this shift strategy. When there are large clusters of closely spaced frequencies, as found, for example, in building models no two frequencies can be found far enough apart for a shift to be performed. If a shift is forced within the convergence radius of a previously converged eigenvalue, the logic of this procedure cannot cope with eigenvalues computed twice. This is the situation described in Ref [4]. It may be overcome by choosing μ between two eigenvalues which have converged to a high tolerance instead of between a converged and an unconverged one.

2.3 LANCZOS QR

The Lanczos QR-method is described in a number of References [6,7,8]. The solution procedure is summarized in Table 3. The original eigenvalue problem is transformed to

$$(\underline{A} - \underline{\lambda} \underline{I}) \underline{Z} = 0 \quad (5)$$

in which $\underline{A}$ is a symmetric, tridiagonal matrix of order m and $\underline{I}$ is the unit matrix. Approximately the lower half of the m eigenvalues computed are useable while the other eigenvalues are unacceptable. Since the formation and the solution of eq.(5) cannot be carried out in primary storage careful planning of secondary storage operations for transforming the original eigenvalue problem, solving the tridiagonal eigenproblem, and transforming the solution vectors $\underline{Z}$ back to the eigenvectors $\underline{\phi}$ is important. The complete set of $\underline{Z}$ -vectors would require m^2 storage spaces. If m is twice the number of required frequencies, this number becomes prohibitively large, thus secondary storage is mandatory. For the computation of each of the m Lanczos vectors $\underline{V}$ the complete blocked, decomposed stiffness matrix $\underline{K} = \underline{L} \underline{D} \underline{L}^T$ has to be passed through the subroutine REDVK during forward reduction and back substitution. This accounts for the major part of the computational effort. While this takes place the computation of the tridiagonal matrix coefficients is being completed. Orthogonalizing and storing of the Lanczos vectors accounts for the moving of approximately $m^2 n$ words. An additional $m \cdot n_b$ words are moved during the retransformation from the $\underline{Z}$'s to the $\underline{\phi}$'s

$$\underline{\phi} = \underline{V} \underline{Z} \quad (6)$$

where $\underline{\Phi}$ and $\underline{V}$ are n by m and $\underline{Z}$ is an m by m matrix. As will be seen in the case studies the formation of the tridiagonal matrix accounts for the largest part of the computational effort and of the input/output activity on secondary storage.

2.4 HOUSEHOLDER QR

The Householder QR-method is similar to the Lanczos method in that it transforms the original eigenvalue problem with the system matrices $\underline{K}$ and $\underline{M}$ to the tridiagonalized problem of eq.(5). The difference is in the size of the tridiagonalized problem: Lanczos operates with m vectors, where m is approximately twice the number of requested eigenpairs while Householder uses all n vectors (see Ref.[1] pp.460-473). The storage required is of the order $n(n+1)/2$. For large models this primary storage requirement cannot be met. Therefore the Householder QR-method in the present form cannot be used for large building type models.

2.5 EXPLOITING MODEL SYMMETRY

There are a number of cases in which the model exhibits at least one symmetry plane (Fig.1). The symmetry is exploited for drastic cost reduction by using a half-model with $\underline{K}_H$ and $\underline{M}_H$. Two eigenproblems have to be solved

$$(\underline{K}_S - \underline{\Omega}_S^2 \underline{M}_S) \underline{\Phi}_S = 0 \quad \text{and} \quad (\underline{K}_A - \underline{\Omega}_A^2 \underline{M}_A) \underline{\Phi}_A = 0 \quad . \quad (7,8)$$

The indices S and A correspond to the symmetry and antisymmetry conditions, respectively, on the symmetry plane. For the model on Fig.1 they are (see Ref.[9])

$$u_x = w_y = w_z = 0 \quad (S) \quad \text{and} \quad u_y = u_z = w_x = 0 \quad (A) \quad . \quad (9)$$

The solution of the two eigenproblems of eq.(7,8) delivers the complete modes of the half model (H) and the reflected model (R)

$$\underline{\Phi} = \begin{bmatrix} \underline{\Phi}_H \\ \underline{\Phi}_R \end{bmatrix} = \begin{bmatrix} \underline{\Phi}_S & \underline{\Phi}_A \\ \underline{\Phi}_S & -\underline{\Phi}_A \end{bmatrix} \quad . \quad (10)$$

When the generalized masses are computed,

$$\underline{M}^* = \underline{\Phi}^T \underline{M} \underline{\Phi} = \begin{bmatrix} 2\underline{\Phi}_S^T \underline{M}_H \underline{\Phi}_S & 0 \\ 0 & 2\underline{\Phi}_A^T \underline{M}_H \underline{\Phi}_A \end{bmatrix} \quad (11)$$

it becomes obvious that no other modes exist.

A time history analysis with loads on the half-model, $\underline{P}_H$, and on the reflected model, $\underline{P}_R$, is carried out by considering the symmetric and the antisymmetric half-model separately. The half-model load components are

$$\underline{P}_S = (\underline{P}_H + \underline{P}_R)/2, \quad \underline{P}_A = (\underline{P}_H - \underline{P}_R)/2, \quad (12)$$

and the results (displacements, accelerations, stresses) are

$$\underline{V}_S = \underline{\Phi}_S \underline{Y}_S(t), \quad \underline{V}_A = \underline{\Phi}_A \underline{Y}_A(t) \quad . \quad (13)$$

The final results for the half-model and the reflected model are obtained by superposition:

$$\underline{V}_H = \underline{V}_S + \underline{V}_A, \quad \underline{V}_R = \underline{V}_S - \underline{V}_A. \quad (14)$$

The reflected model is found from the half-model by mirror-imaging the nodes and elements on the symmetry plane.

The savings of solving the two half-models of eq.(12) are dramatic in light of n , m_k and m all being approximately half of the full model.

3. BUILDING MODELS

3.1 MODEL CHARACTERISTICS

The building models (see Table 4) which have been analyzed consist of truss, beam, plate, and uncoupled and coupled spring elements. Model 1 (Table 4) is an internal structure with additional pipe elements. It has been used for checking solution times of the various solution methods mentioned in this paper. The other models are typical building models with a large number of equations and a large half-bandwidth. In the building models only the translational degrees of freedom carry any mass. Approximately five percent of the total degrees of freedom do not carry any stiffness. This is due to the lack of rotational stiffness normal to the plate surface. Of the 2754 total degrees of freedom of model 5, there are 1377 mass dof, and 2636 stiffness dof. The excess dof are automatically restrained.

3.2 COMPARISON OF EIGENSOLUTIONS

In Table 4 only two solution methods are compared, the Lanczos QR-method (LQR) and the subspace iteration with progressive forward shifting (SPFS). From the comparison of models 5 through 8 it is apparent that LQR is superior to SPFS even when only 10 frequencies are being computed. This is true for a small field length (work area 29500 words) and a large field length (work area 55000 words). The LQR total solution time is only between 50 and 60 percent of the SPFS time. This is the reason for favoring the application of the LQR solution method. All solution results have been checked with STARDYNE results for accuracy by comparing frequencies and mode shapes, generalized weights, composite damping, modal participation factors and modal weights.

3.3 COMPUTATIONAL PERFORMANCE

The performance characteristics can be examined from the CPA, I/O, CM, SS and wall clock time readings. Models 2 and 3 differ in total dof by 14 percent (based on the smaller model) and have the same half-bandwidth. For the larger model 50 percent more modes and frequencies have been requested. All performance parameters have more than doubled. An important performance figure is the ratio of wall clock time over total solution time. This ratio is approximately 10 and more for the LQR method.

4. CONCLUSIONS

Of all the eigensolution algorithms considered in this paper the Lanczos QR-method is the most promising one. By further reduction of the amount of data transfer between primary and secondary storage, particularly during tridiagonalization, the method can be extended for extremely large models. The most important area of urgently needed improvements is the reduction of the time the computer run is resident in the computer (wall clock time).

5. REFERENCES

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Table 1 - Subspace Iteration with User-Initiated Shift

Step	Operation	Computation
1	Establish frequency range $\mu_{\min} = \omega_{\min}^2, \mu_{\max} = \omega_{\max}^2$	$\hat{K}_{\max} = K - \mu_{\max} M$ $\hat{K}_{\min} = K - \mu_{\min} M$
2	Count number of frequencies in range by $\hat{K} = L D L^T$	$\Delta m = m_{\max} - m_{\min}$
3	Perform shift $\mu \approx \frac{1}{2}(\mu_{\min} + \mu_{\max})$	$\hat{K} = K - \mu M$
4	Factorize $\hat{K}$	$\hat{K} = L D L^T$
for iteration k:		
5	Set trial vectors X_k Compute inertia forces Y_k	$Y_k = M X_k$
6	Solve for improved trial vectors in subblocks a,...,g	$\hat{K} \begin{bmatrix} \tilde{X}_a \\ \vdots \\ \tilde{X}_g \end{bmatrix} = \begin{bmatrix} Y_a \\ \vdots \\ Y_g \end{bmatrix}$
7	Form subspace stiffness	$\hat{K}^* = \tilde{X}_k^T \hat{K} \tilde{X}_k$
8	Improved inertia forces	$\tilde{Y}_k = M \tilde{X}_k$
9	Form subspace mass	$M^* = \tilde{X}_k^T M \tilde{X}_k$
10	Solve subspace eigenvalue problem with Jacobi Method	$[(K^* - \lambda M^*) - Q^2 M^*] Q^* = 0$
11	Compute improved vectors	$X_k = \tilde{X}_k Q^*$
12	Check tolerance for all eigen- values $\omega_j, j=1, \dots, m$	$\epsilon_j = \frac{\omega_{j,k-1}^2 - \omega_{j,k}^2}{\omega_{j,k}^2} \leq \text{tol}$
13	If tolerance is not met got to 5	$X_k \rightarrow X_{k+1}$
14	Complete solution	$\omega_{j,k} \rightarrow \omega_j, X_k \rightarrow \Phi$

Table 2 - Subspace Iteration with Progressive Forward Shifting

Step	Operation	Computation
1	Perform shift	$\hat{K} = K - \mu M$
2	Factorize $\hat{K}$	$\hat{K} = L D L^T$
for iteration k:		
3	Using trial vectors X_k compute inertia forces Y_k	$Y_k = M X_k$
4	Solve for improved trial vectors	$\hat{K} \tilde{X}_k = Y_k$
5-10	see steps 7 through 12 in Table 1 Form and solve transformed and shifted eigenvalue problem, compute improved vectors and check tolerances	
11	Replace converged eigenvectors with random vectors, orthogonalize with respect to converged vectors to form new trial subspace, X_{k+1}	$X_k \rightarrow X_{k+1}$
12	Compute new shift shift strategy determines whether to go to 1 or to go to 3.	μ_{new}
13	Complete solution	$\omega_{j,k} \rightarrow \omega_j, X_k \rightarrow \Phi$

Table 3 - Lanczos QR 1)

Step	Operation	Computation
1	Factorize $\underline{K}$	$\underline{K} = \underline{L} \underline{D} \underline{L}^T$
for each vector $j \quad j=1, \dots, m$		
2	Generate random vector $\underline{X}_j$ and compute inertia force $\underline{Y}_j$	$\underline{Y}_j = \underline{M} \underline{X}_j$
3	Compute Lanczos vector $\underline{\tilde{V}}_j$	$\underline{K} \underline{\tilde{V}}_j = \underline{Y}_j$
4	Normalize Lanczos Vector	$\underline{V}_j = \frac{\underline{\tilde{V}}_j}{(\underline{\tilde{V}}_j^T \underline{M} \underline{\tilde{V}}_j)^{1/2}}$
5	Check orthogonality of trial vector with all previously computed vectors $i=1, \dots, j-1$	$\underline{M}_{ij}^* = \underline{V}_i^T \underline{M} \underline{V}_j$
6	If not orthogonal, reorthogonalize iteratively ($k \leq 14$ iterations)	$\underline{\tilde{V}}_j^k = \underline{\tilde{V}}_j^{k-1} - \sum_{i=1}^{j-1} \underline{M}_{ij}^* \underline{V}_i$
7	Normalize orthogonal Lanczos Vector	$\underline{V}_j^k = \frac{\underline{\tilde{V}}_j^k}{[(\underline{V}_j^k)^T \underline{M} \underline{V}_j^k]^{1/2}}$
8	Compute second Lanczos Vector	$\underline{K} \underline{W}_j = \underline{V}_j^k$
9	Compute off-diagonal coefficient	$\underline{\beta}_j = \underline{W}_j^T \underline{M} \underline{V}_{j-1}$
10	Compute diagonal coefficient	$\underline{\alpha}_j = \underline{W}_j^T \underline{M} \underline{W}_j$
11	Compute new Lanczos Vector	$\underline{\tilde{V}}_{j+1} = \underline{W}_j - \underline{\alpha}_j \underline{V}_j - \underline{\beta}_j \underline{V}_{j-1}$
12	Normalize new Lanczos Vector	$\underline{V}_{j+1} = \frac{\underline{\tilde{V}}_{j+1}}{(\underline{\tilde{V}}_{j+1}^T \underline{M} \underline{\tilde{V}}_{j+1})^{1/2}}$
13	Solve tridiagonalized m by m eigenproblem	$(\underline{A} - \underline{\lambda} \underline{I}) \underline{Z} = \underline{0}$
14	Transform back to original m by n vector space from m by m tridiagonalized problem space using Lanczos vectors	$\underline{\omega}_j^2 = \frac{1}{\underline{\lambda}_j}$ $\underline{\Phi} = \underline{V} \underline{Z}$
15	Check tolerances (eq.27a, Ref.[7])	$\underline{\epsilon}_j \leq \text{tol}$

1) Ref.[7], pp.35-43

Fig.1 - Model with one Symmetry Plane

Table 4 - Summary of Eigensolution Computations

Model name	Kühler KKP2	Pumpengebäude KKE		GKN2	Notstrom- dieselgeb. Anlage	Notspeisegebäude Grohnde			
Model number	1	2	3	4	5	6	7	8	
Number of equations, m	338	2172	2485	3510	2754				
half-bandwidth of $\underline{K}$, m_k	54	262	260	678	462				
number of blocks n_b	2	22	31	93	89				
number of equations in a block, n_{eqb}	263	103	82	38	31				
number of frequencies requested n_f	10	100	150	212	10	10	10	10	
number of vectors in eigenvalue problem m	30	210	310	434		30			
method of analysis	LQR	LQR	LQR	LQR	SPFS	LQR	SPFS	LQR	
type of computer used	C720	C176	C176	C175	C176	177400	261200	261200	
max. field length (words)	177400	261200	261200	261200	177400	177400	906	261200	
CPA central processor (sec)	16	1702	3610		1222	646	516	568	
I/O input/output (sec)	23	1889	3860		908	648	6067	538	
CM central memory (sec)	107	16405	34115		6661	4189	7489	4977	
SS system seconds total (sec)	146	19997	41586		8791	5484	2545	6084	
wall clock time (sec)	319	8450	17287		4273	2943		2461	
time checks on eigensolution (sec)									
LQR: stiffness factorization	3	26	33	513		115		85	
tridiagonalization	26	581	1115	5864		144		140	
eigenvalue calc.	5	60	242	1514		1		1	
eigenvector calc.	4	82	203	1689		3		2	
total	39	749	1594	9582		263		229	
total eigensolution (sec)				10732	567		413		
total solution (sec)				10844	609	321	451	282	

LQR = Lanczos QR-method; SPFS = Subspace iteration with progressive forward shifting.

C = Cyber.