A block Lanczos method with spectral transformations for natural vibrations and seismic analysis of large structures in SCAD software

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Abstract

A powerful eigenvalue extraction method for natural vibration analysis of large-scale structures is presented. This method is based on a block Lanczos algorithm with shift implementation [4] and has four modes of operation: modal mode, interval mode, seismic mode and verification mode. The modal mode is developed to extract the first n required eigenpairs. The interval mode means the extracting of all eigenpairs whose frequencies fall into an interval $[a,b]$. The seismic mode is intended for extracting eigenpairs while ensuring that a required sum of modal masses be provided for all seismic input directions. The verification mode is used to detect hard-to-find errors of a finite element model, such as a local and global dimensional instability, lack of supports and so on. The shift technique is applied to split the frequency interval into small subintervals and restricts the growth of the computation effort for large-scale dynamic problems. The sparse direct solver, based on multifrontal technique, is used to factor the stiffness matrix. It provides not only a faster factoring procedure, but fast forward-back substitutions during repeated Lanczos steps. The performance of this method is compared here with that of different solvers. Its robustness and efficiency is confirmed by numerous examples.

Keywords: eigenvalue, shift, trust interval, block, multifrontal

1. Introduction

Recently, large-scale problems with large number of eigenpairs arise more and more often. Therefore it requires robust and fast methods for eigenvalue analysis to be developed.

The great number of eigenpairs is needed often for seismic analysis when a lot of low vibration modes are local and/or do not make a representative contribution to the seismic response of a structure in question. It is very difficult to ensure the sufficient percentage of the sum of modal masses [1], [3], [9] along all or some principal seismic directions.

The conventional procedure of extracting low vibration modes (a modal mode) consists of following: the user assigns the number of desired modes, runs the analysis and checks the sum of modal masses in each direction. If the sum of modal masses is insufficient, the user increases the required number of modes and runs the calculation again. And so on. For "hard" problems this procedure is usually repeated multiple times. It is not an efficient way to solve seismic problems. The seismic mode (regime) of a block Lanczos method proposed here is based on shift implementation and a posteriori bounding of residual [2], [4], and it allows us to obtain all modes, provide the required sum of modal masses during one run of algorithm and avoid time-consuming attempts which are typical for conventional approaches.

The design of nuclear power plants and other industrial buildings often requires to extract all natural vibration frequencies belonging to a given frequency interval $[a,b]$. The interval mode of the proposed block Lanczos method, based on Sturm check sequences and a shift technique, implements this approach.

A considerable effort and design time are spent to detect errors in large-scale finite element models, like local and global dimensional instability, lack of supports and so on. The verification mode proposed here, one based on a shift technique, helps detect these hard-to-find errors. This approach has proved to be better than an analysis based on singularities detected during the matrix factoring.

Numerical examples presented here illustrate the capabilities of the proposed method.

2. Block Lanczos method with spectral transformations

The Lanczos method [5], [6], [7] is recognized as a most powerful tool for extraction of large number of eigenpairs in large-scale problems of structural mechanics. The stability of its computational process is ensured by a selective or/and partial re-orthogonalization [5], [6], [7]. The experience of authors [3] indicates that the selective re-orthogonalization based on Paige's theorem, is efficient only for relatively short Lanczos processes when the number of generated Lanczos vectors is not too great. For long Lanczos processes the selective re-orthogonalization fails to succeed. On the contrary, the partial reorthogonalization [7], [8] keeps Lanczos vectors highly orthogonal and ensures a highly stable computation even for long Lanczos processes which generate 300-700 and more Lanczos vectors. Therefore we employ the block version of partial re-orthogonalization [4].

Conventional algorithms of Lanczos method possess the following disadvantage when the large-scale problems containing 60 000 - 500 000 and more equations are to be solved: at each step of Lanczos vector generation it is necessary to make the forward-back substitutions only for a single right-side vector (r. s. v.). Due to this a lot of computation time is spent for input-output (I/O) operations because the upper part of the factored matrix $\mathbf{U}$, where $\mathbf{K} = \mathbf{L}\mathbf{U}$ and $\mathbf{K}$ is a stiffness matrix, must be read twice block-by-block from a secondary storage (disk) per each Lanczos vector.

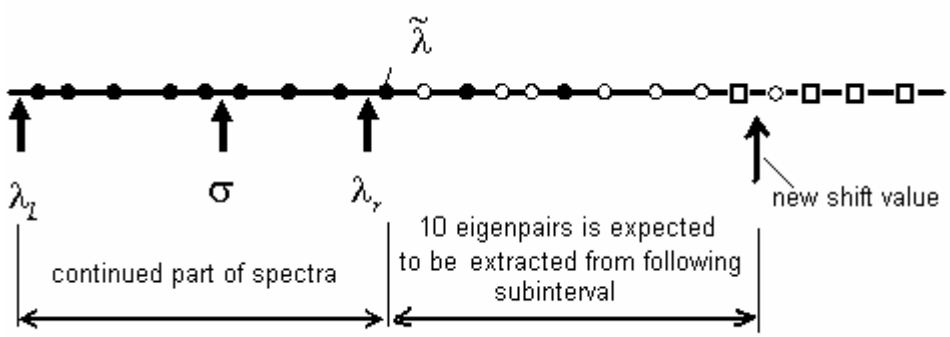

Fig.1 Typical distribution of eigenvalues, Ritz approximations and coarse approximations. ● - eigenpairs; o - Ritz pairs; □ - coarse approximations

The second problem is related to a drastic increase of amount of operations when the dimension of Krylov subspace (number of generated Lanczos vectors) is big enough (usually exceeds ~100).

The block version of Lanczos algorithm is intended to reduce the I/O effort.

Spectral transformations are implemented to split the long Lanczos process into a few relatively short ones. It reduces essentially the computation time when a large number of eigenpairs (100 - 1000 and more) are required.

The original natural vibration problem is as follows:

$$\mathbf{K}\varphi - \lambda\mathbf{M}\varphi = 0 \tag{1}$$

where $\mathbf{K}$ is a positive definite symmetrical stiffness matrix and $\mathbf{M}$ is a positive definite or semi-definite lumped or consistent mass matrix, λ, φ is an eigenpair.

The idea of the shifted block Lanczos algorithm [4] is adopted as a basis for the algorithm presented here, although many details have been modified and adjusted to peculiarities of structural mechanics problems.

The basic algorithm of the block Lanczos method with spectral transformations is presented below.

1. $\lambda_l = \lambda_r = \sigma = a$, where λ_l, λ_r are left and right boundaries of the trust interval, a is the leftmost boundary of the interval $[a,b]$, σ is a shift value. The trust interval contains only converged Ritz pairs (we refer to them as eigenpairs) and does not have any missed ones, that is, all eigenpairs from trust interval $[\lambda_l, \lambda_r]$ are thought to have been extracted. Set the block size p (usually $p = 3$) and $in = 1$.
2. External loop: continue solution till all required eigenpairs are extracted with a given accuracy.
3. Set the start block $\mathbf{Q}_0 = \left\{\mathbf{q}_1^0, \mathbf{q}_2^0, , , \mathbf{q}_p^0\right\} = 0$ and $\mathbf{R}_1 = \left\{\mathbf{r}_1^0, \mathbf{r}_2^0, ..., \mathbf{r}_p^0\right\}$, where all vectors in block $\mathbf{R}_1$ are linearly independent. Then: $\mathbf{Q}_1\mathbf{B}_1 = \mathbf{R}_1$, where $\mathbf{B}_1$ is an upper triangle matrix $p \times p$ and $\mathbf{Q}_1^T\mathbf{M}\mathbf{Q}_1 = \mathbf{I}$. It is a matrix form of the block Gram-Schmidt orthogonalization algorithm, which in this article differs from that presented in [4]. The size of blocks $\mathbf{Q}, \mathbf{R}$ is $N \times p$ where N is the number of equations of (1).
4. If $in > 1$, modify $\sigma = \lambda_l + \Delta\lambda$, where the choice of $\Delta\lambda$ is based on estimation of Ritz pairs (see below). If $\sigma \neq 0$, perform the factoring of $\mathbf{K}_\sigma = \mathbf{K} - \sigma\mathbf{M} = \mathbf{L}_\sigma\mathbf{U}_\sigma$.
5. Internal loop: $j = 1,2,...,$
6. Calculate:

$$\begin{aligned} &\mathbf{K}_\sigma\mathbf{U}_j = \mathbf{M}\mathbf{Q}_j \Rightarrow \mathbf{U}_j \\ &\mathbf{U}_j := \mathbf{U}_j - \mathbf{Q}_{j-1}\mathbf{B}_j^T \\ &\mathbf{A}_j = \mathbf{U}_j^T\mathbf{M}\mathbf{Q}_j \\ &\mathbf{R}_{j+1} = \mathbf{U}_j - \mathbf{Q}_j\mathbf{A}_j \end{aligned} \tag{2}$$

7. $\mathbf{Q}_{j+1}\mathbf{B}_{j+1} = \mathbf{R}_{j+1}$, where $\mathbf{Q}_{j+1}^T\mathbf{M}\mathbf{Q}_{j+1} = \mathbf{I}$
8. Update the block triangle matrix

$$\mathbf{T}_j = \begin{Bmatrix} \mathbf{A}_1 & \mathbf{B}_2 & & & \\ \mathbf{B}_2^T & \mathbf{A}_2 & \mathbf{B}_3 & & \\ & \mathbf{B}_3^T & \mathbf{A}_3 & \mathbf{B}_4 & \\ \dots & \dots & \dots & \dots & \dots \\ & & & \mathbf{B}_j^T & \mathbf{A}_j \end{Bmatrix} \tag{3}$$

9. Solve the reduced eigenvalue problem

$$\mathbf{T}_j\mathbf{S}_j = \mathbf{\Theta}_j\mathbf{S}_j \tag{4}$$

10. Compute the precision of Ritz pairs using a posteriori boundary of residual [2],[4]:

$$\left\|\mathbf{M}\mathbf{K}_\sigma^{-1}\mathbf{M}\mathbf{y}_i - \mathbf{M}\mathbf{y}_i\theta_i\right\|_{M^{-1}} = \left\|\mathbf{B}_{j+1}\mathbf{E}_j^T\mathbf{s}_i\right\|_2 = \beta_i^j,\ i = 1,2,...,j \tag{5}$$

where $\mathbf{Y}_j = \left\{\mathbf{y}_1^j, \mathbf{y}_2^j, ..., \mathbf{y}_j^j\right\} = \mathbf{Q}_j\mathbf{S}_j$. The Ritz pair is taken as converged, if $\frac{\beta_i^j}{\left(\theta_i^j\right)^2} \le tol$, where $\left|\lambda_i - \nu_i^j\right| \le \frac{\beta_i^j}{\left(\theta_i^j\right)^2}$ and λ_i is an exact eigenvalue, ν_i^j is an approximation at the Lanczos step j, tol is an adopted tolerance (usually $1.0\times10^{-4} \div 1.0\times10^{-8}$. We provide the following

classification: if $\frac{\beta_i^j}{\left(\theta_i^j\right)^2} \le tol$ then it is a converged eigenpair; if $tol < \frac{\beta_i^j}{\left(\theta_i^j\right)^2} \le 1.0\times10^{-2}$ then it is a Ritz pair; if $\frac{\beta_i^j}{\left(\theta_i^j\right)^2} > 1.0\times10^{-2}$ then it is a coarse approximation (see Fig.1).

11. Break the internal iteration loop at j, if:
    - $(in=1)\wedge(j \ge NL)$, where $NL \cong 150-200$ is the maximal number of Lanczos vectors
    - $(in>1)\wedge\left[n_c^{in} \ge \left(Z(\sigma)-n_{def}\right)\right]$, where n_c^{in} is the number of converged modes at the given step in of the external loop, n_{def} is the number of eigenpairs already found, $Z(\sigma)$ is the number of negative signs detected on the diagonal of $\mathbf{U}_\sigma$.

    These conditions being satisfied ensures that the skipped eigenpairs do not fall into the interval $[\lambda_l, \sigma]$.

    If the internal loop is interrupted, go to step 14.
12. If the orthogonality between Lanczos vectors is less than required, perform a partial re-orthogonalization according with [4] – corrected matrices $\mathbf{Q}_{j+1}, \mathbf{R}_{j+1}, \mathbf{B}_{j+1}$ are the result of it.
13. $j{+}{+}$, go to 5
14. Evaluate the eigenvectors for all eigenvalues enclosed in the interval $[\lambda_l, \tilde{\lambda}]$ (see Fig.1), where $\tilde{\lambda}$ is a largest eigenvalue from the continuous part of the spectrum. In the seismic mode, calculate the sum of modal masses in each principal direction [1], [9].
15. Evaluate a new approximation of $\Delta\lambda$ so that the number of converged eigenvalues, Ritz and coarse approximations, located to the right of $\tilde{\lambda}$, be equal to the expected number of eigenpairs which we want to obtain from the next trust subinterval (see Fig.1). Usually this value is adopted to be 15-20 that corresponds to about 100-150 maximal number of Lanczos vectors. Evaluate λ_r and put $\lambda_l = \lambda_r$ to the next shift interval.
16. In the modal, interval and verification modes: if $n_{def} \ge n_{req}$, where n_{req} is the required number of eigenpairs enclosed in the interval $[a,b]$ and n_{def} is the number of eigenpairs obtained and enclosed in the interval $[a, \lambda_r]$, break the external loop and go to step 17. In the seismic mode: break the external loop and go to step 17, if the sum of modal masses for all converged modes reaches the accepted values (default: $\sum m_x = \sum m_y = 90\%,\ \sum m_z = 75\%$). Otherwise (no finish criterion is satisfied), $in{+}{+}$ and go to step 2.
17. Evaluate the precision for each eigenpair:

$$prec_i = \frac{\left\|\mathbf{y}_i - \lambda_i \mathbf{K}^{-1}\mathbf{M}\mathbf{y}_i\right\|_2}{\left\|\mathbf{y}_i\right\|_2},\ i = 1,2,...,n_{def} \qquad (6)$$

This algorithm ensures that the skipped eigenpairs do not fall into the interval $[a, \sigma_{last}]$ where σ_{last} is the last shift value.

The algorithm presented above implements the modal and interval modes. In addition, when the interval mode is used, we define the number of eigenvalues enclosed in the given interval $[a,b]$:

$$n_{def} = Z(\sigma = b) - Z(\sigma = a) \qquad (7)$$

The initial shift value is taken as $\sigma = a$.

In the seismic mode the computation stops as soon as the required sum of modal masses is reached.

In the verification mode, a small negative shift is implemented to avoid a singularity caused by potential errors in the computation model.

3. Numerical results

3.1. The modal mode

The modal mode of the proposed method is illustrated by the following example. The model of a multi-storey building contains 19 409 nodes, 19 456 finite elements and 115 362 equations (see Fig. 2).

The comparison of computation time vs. the number of required modes (modal mode) for different methods is presented in Table 1. The subspace iteration (SI), block subspace iteration (BSI), a conventional Lanczos method (LM) and the block Lanczos method with spectral transformations (BLST) proposed here are presented. A Pentium-III computer (Intel-1000MHz processor, 512 MB RAM) is used. The precision of all obtained eigenpairs estimated by (6) is not worse than 1.0×10^{-04}.

The block subspace iteration method has been developed according to [9] and is presented in [3]. The conventional Lanczos method has been developed according to [5], [7] and is presented in [3]. This example illustrates a typical performance of these methods. It can be clearly seen that the BSI method is preferable to SI. If the factored stiffness matrix can fit in RAM, then the Lanczos method is essentially faster than BSI. The more the number of required modes, the bigger the advantage of the Lanczos method.

Otherwise, if the size of the factored stiffness matrix is too big for it to be allocated in RAM, while the number of required modes is not so big (about 10 - 50), the BSI method usually happens to be more efficient than that of Lanczos due to blocking of I/O operations during forward-back substitutions (see examples from [3]).

The BLST method is essentially faster than other considered methods, especially when the number of required modes is large. The size of Krylov subspace (number of Lanczos vectors) remains relatively small during spectral transformations. An appropriately chosen shift divides the required interval into a sequence of non-overlapped trust subintervals. We pass from a preceding subinterval to the following one till the required number of modes are converged or the proper sum of modal masses is achieved. The required interval is a trust interval too, because it is a sum of adjacent non-overlapped trust subintervals. Inasmuch as each modification of shift leads to the factoring of matrix $\mathbf{K}_\sigma = \mathbf{K} - \sigma\mathbf{M}$, the fast multi-frontal solver with sparse reordering plays an important role.

The last row of Table 1 illustrates great capabilities of the BLST method presented here.

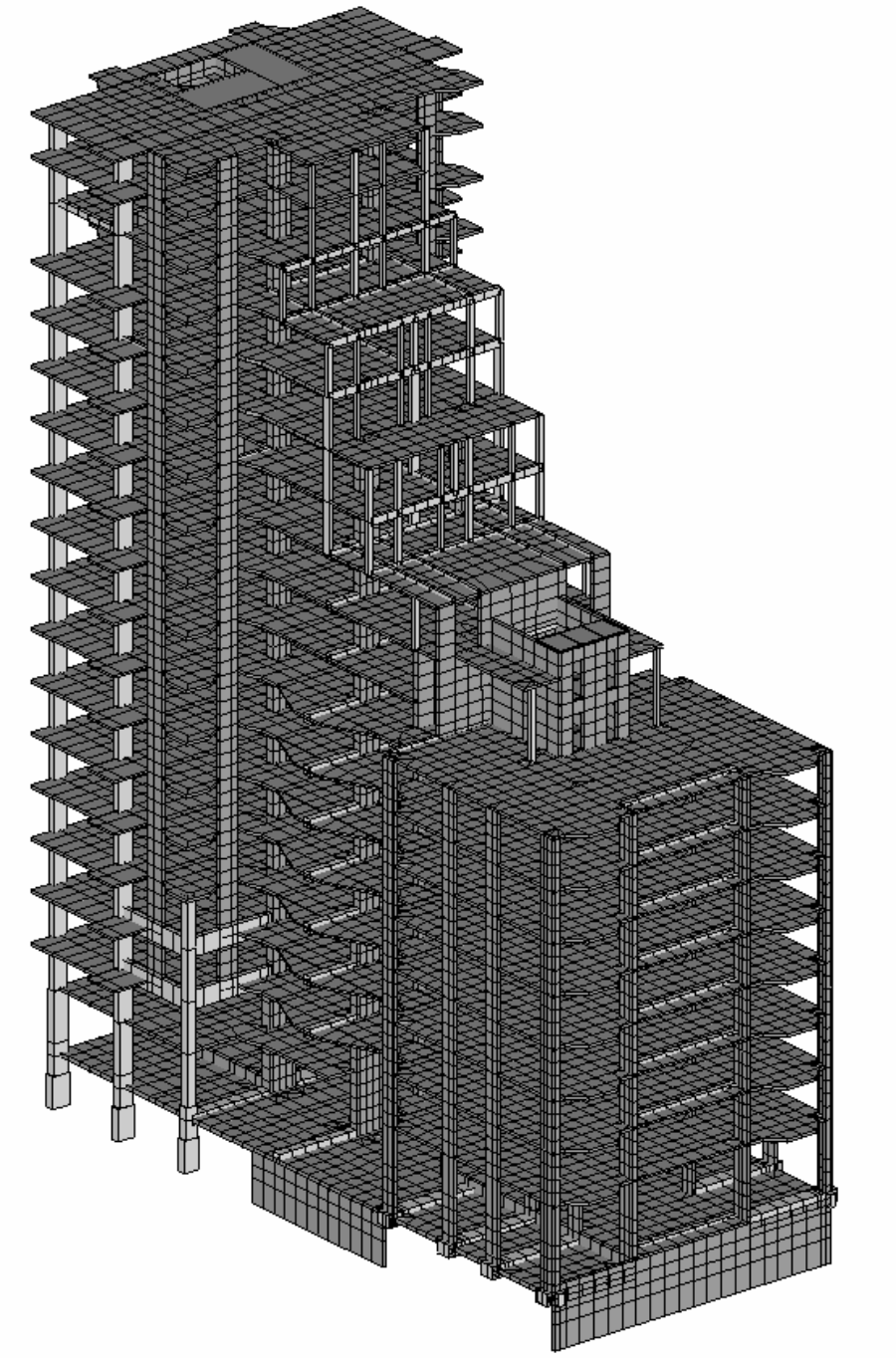

Fig. 2 A multi-storey building

Table 1: Comparison of computation time for different methods. A multi-storey building (Fig.2)

Number of required modes	Subspace iterations	Block subspace iterations [3]	Lanczos method [3]	Block Lanczos method with spectral transformations
25	2 h 28 min 31s	1 h 49 min 38 s	54 min 24 s	38 min 14 s
50	5 h 18 min 33 s	3 h 06 min 16 s	1 h 22 min 37 s	55 min 56 s
100	—	—	2 h 22 min 14 s	1 h 52 min 14 s
1 000	—	—	—	11 h 25 min 02 s

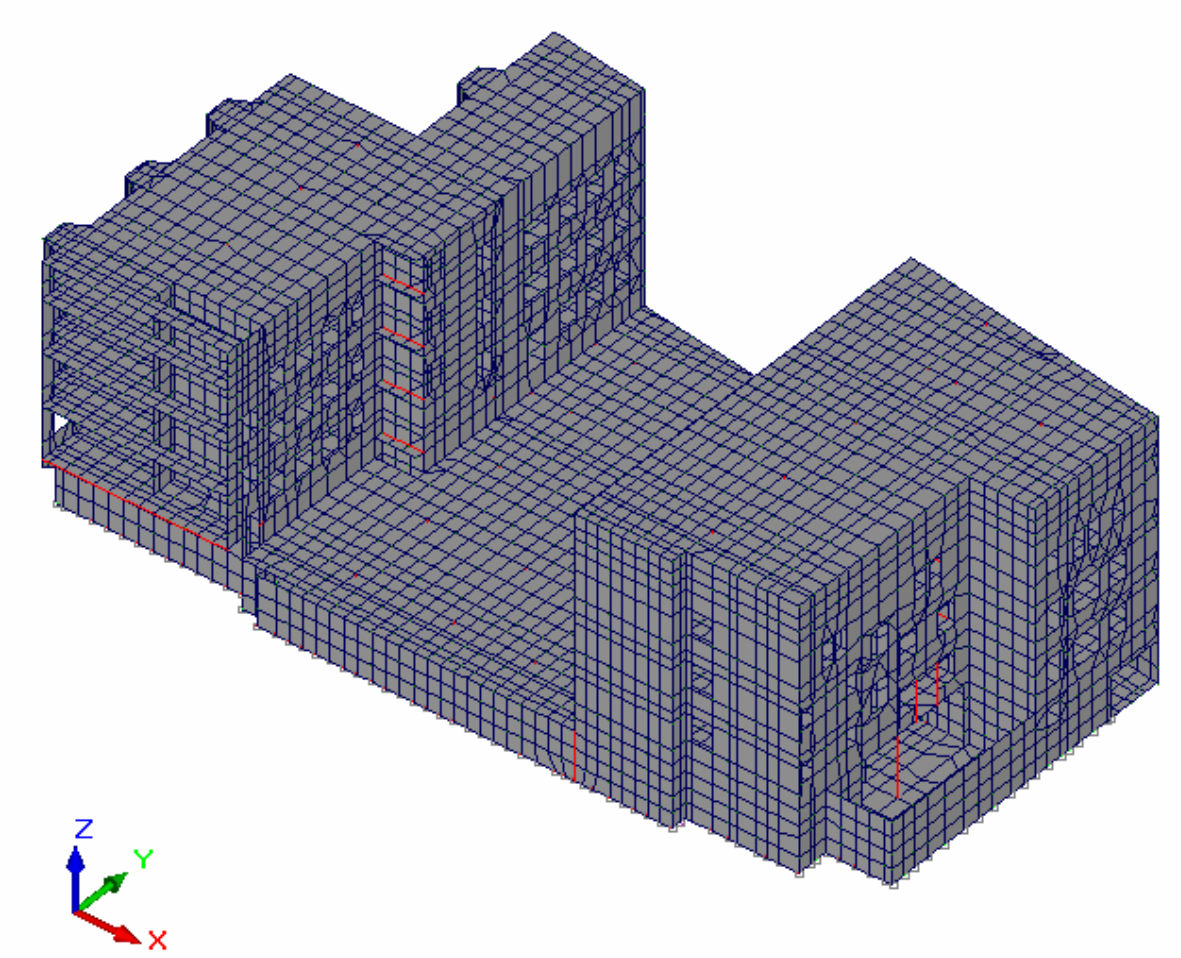

Fig. 3 An industrial building. The frequency band of equipment is 8 to 20 Hz.

3.2. The interval mode

The example shown in Fig. 3 illustrates the interval mode of the block Lanczos method with spectral transformations.

This model contains 10 439 nodes, 11 431 finite elements and 60 760 equations. The frequency band of equipment is 8 to 20 Hz.

First of all, the proposed algorithm evaluates the number of eigenpairs enclosed in the interval [8, 20] Hz by (7). The first Sturm sequence check (SSCH) is performed for the shift corresponding to the top boundary of the frequency (20 Hz). The second SSCH is performed for the bottom boundary (8 Hz). The required number of eigenpairs is 97.

Three subintervals are required to extract 97 eigenpairs. The first subinterval is [8, 13.837] Hz ($\sigma = 8$ Hz, 46 eigenpairs have converged), the second one is [13.837, 18.578] Hz ($\sigma = 16.343$ Hz, 41 eigenmodes have converged) and the third one is [18.578, 22.624] Hz ($\sigma = 20.807$ Hz, 39 eigenpairs have converged). In fact, the algorithm evaluates 126 eigenpairs from the interval [8, 22.624] Hz that is wider than required because the left boundary of each trust subinterval must match the right boundary of its preceding subinterval. Otherwise, the continuity of the spectrum is not safely guaranteed.

Four factorings of matrix $\mathbf{K}_\sigma = \mathbf{K} - \sigma\mathbf{M}$ are required.

The precision of the extracted eigenpairs estimated by (6) is not worse than $1.0e-08$. It is a very high accuracy, and we believe that the proposed method has given nearly exact eigenpairs of the presented finite-element model.

The computation time is 45 min 45 s on a Pentium-III computer (Intel-1000 MHz processor, 512 MB RAM).

3.3. The seismic mode

Big difficulties often arise in the seismic analysis when a lot of eigenpairs are required to achieve a good sum of modal masses. The following examples illustrate this problem (see Tables 2,3) and capabilities of the proposed method.

Table 2: Sum of modal masses versus number of extracted eigenmodes. The model of church (Fig.4)

Number of modes	$\sum m_X$,%	$\sum m_Y$,%	$\sum m_Z$,%
10	50.0	51.9	0.0
50	58.2	77.3	5.1
100	68.4	84.5	13.9
300	95.4	95.2	74.3
638	97.9	97.3	90.0

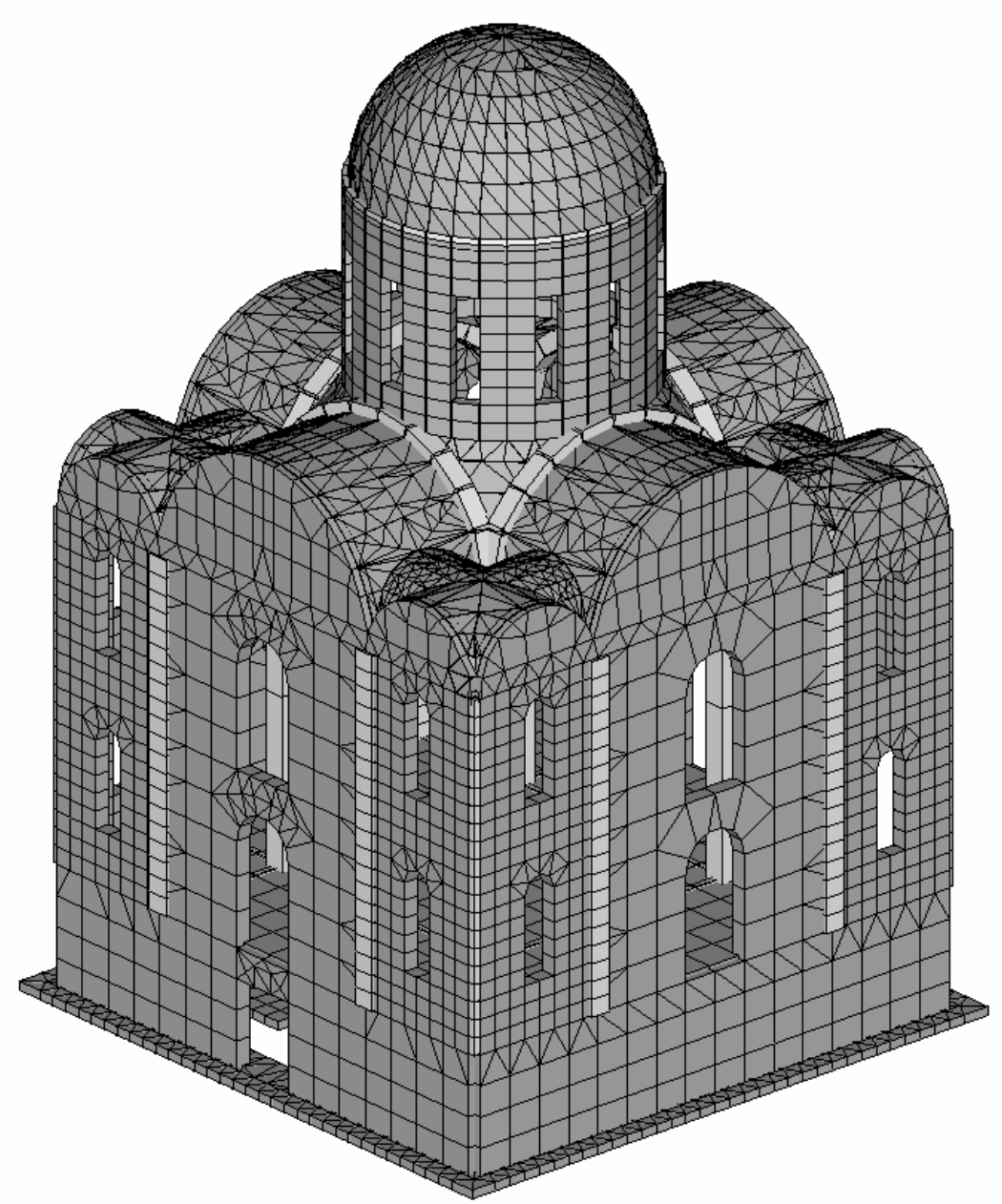

Fig. 4 The model of a church (4 525 nodes, 6 520 finite elements, 27 138 equations)

Table 3: Sum of modal masses vs. number of extracted eigenmodes. A multi-storey building (Fig.5)

Number of modes	$\sum m_X$,%	$\sum m_Y$,%	$\sum m_Z$,%
10	79.6	80.7	7.5
50	83.5	84.5	47.6
100	84.9	88.5	63.8
300	91.6	92.3	82.1
924	94.8	95.6	90.0

The required sum of modal masses is taken as 90% in each principal direction (in compliance with UBC-97, PS-92 and Eurocode-8 seismic codes).

The Church problem requires 638 eigenmodes to satisfy the seismic codes mentioned above. The second problem (a multi-storey building) requires 924 eigenmodes. In fact, 1051 eigenpairs have been extracted for the second problem and 20 trust subintervals have been created. The precision of eigenvectors is not worse than $1.0e-08$. The computation time is 13 h 52 min on a Pentium-III computer (Intel-1000MHz processor, 512 MB RAM).

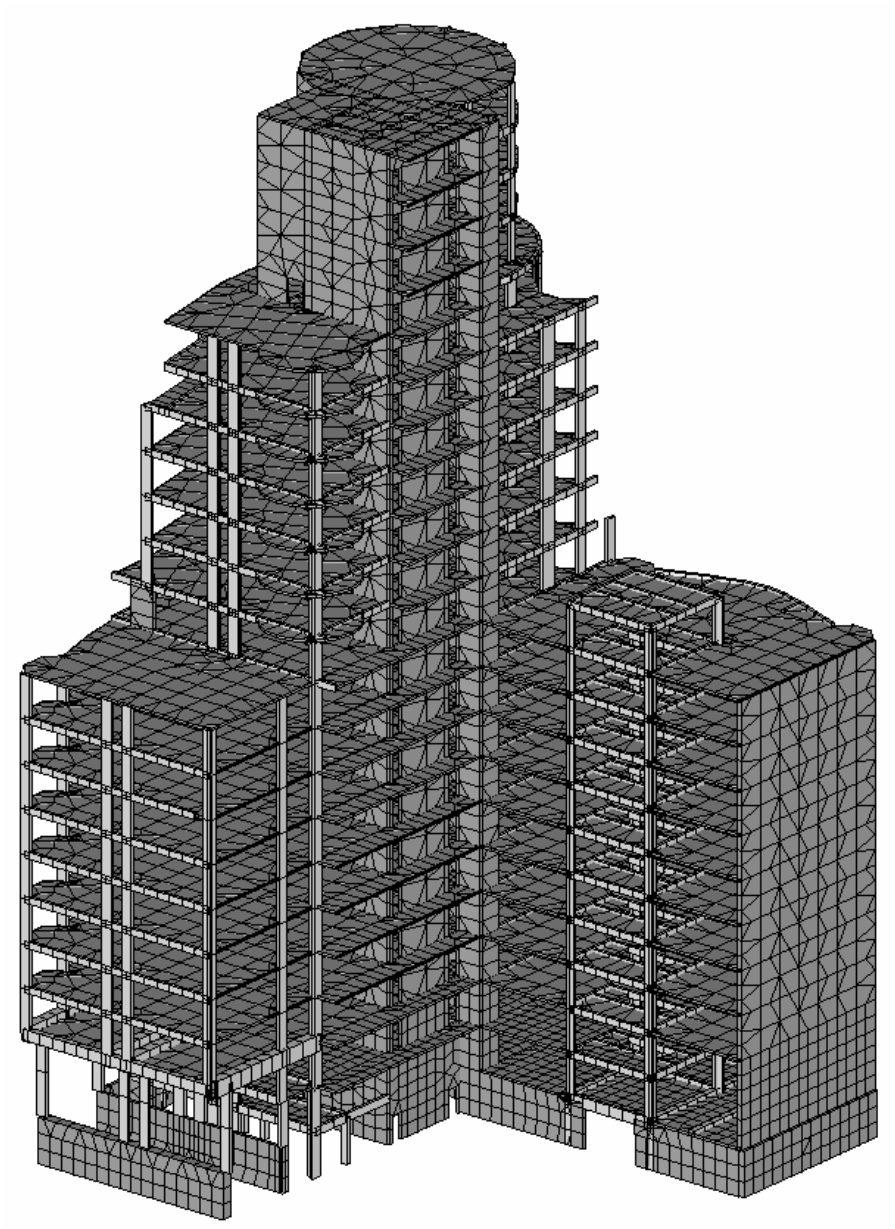

Fig. 5 A multi-storey building (20 285 nodes, 29 932 finite elements, 119 874 equations)

3.4. The verification mode

This mode of the method allows us to detect hard-to-find errors of computational models like local or global dimensional instability, lack of supports and so on.

A small negative shift is implemented to avoid the singularity caused by potential errors in computation model. An example taken from real engineering practice is presented in Fig. 6. First frequencies are shown in Table 4.

The modes 1-6 have nearly zero frequencies. This indicates a dimensional instability. Indeed, the analysis of eigenmodes detects an unconstrained part in the structure which has six modes of free rigid body motion. The first mode is presented in Fig. 7.

Table 4: Low frequencies of a multi-storey building

Number	Frequency, Hz	Comments
1	-8.228e-006	Free rigid body motion of unconstrained part of structure. Mode 1 is presented in Fig. 7
2	-2.104e-006	
3	2.62e-006	
4	3.172e-006	
5	4.257e-006	
6	5.623e-006	
7	0.5181	The bottoms of columns are not constrained - see Fig. 8
8	0.6726	
9	0.986	
10	1.042	

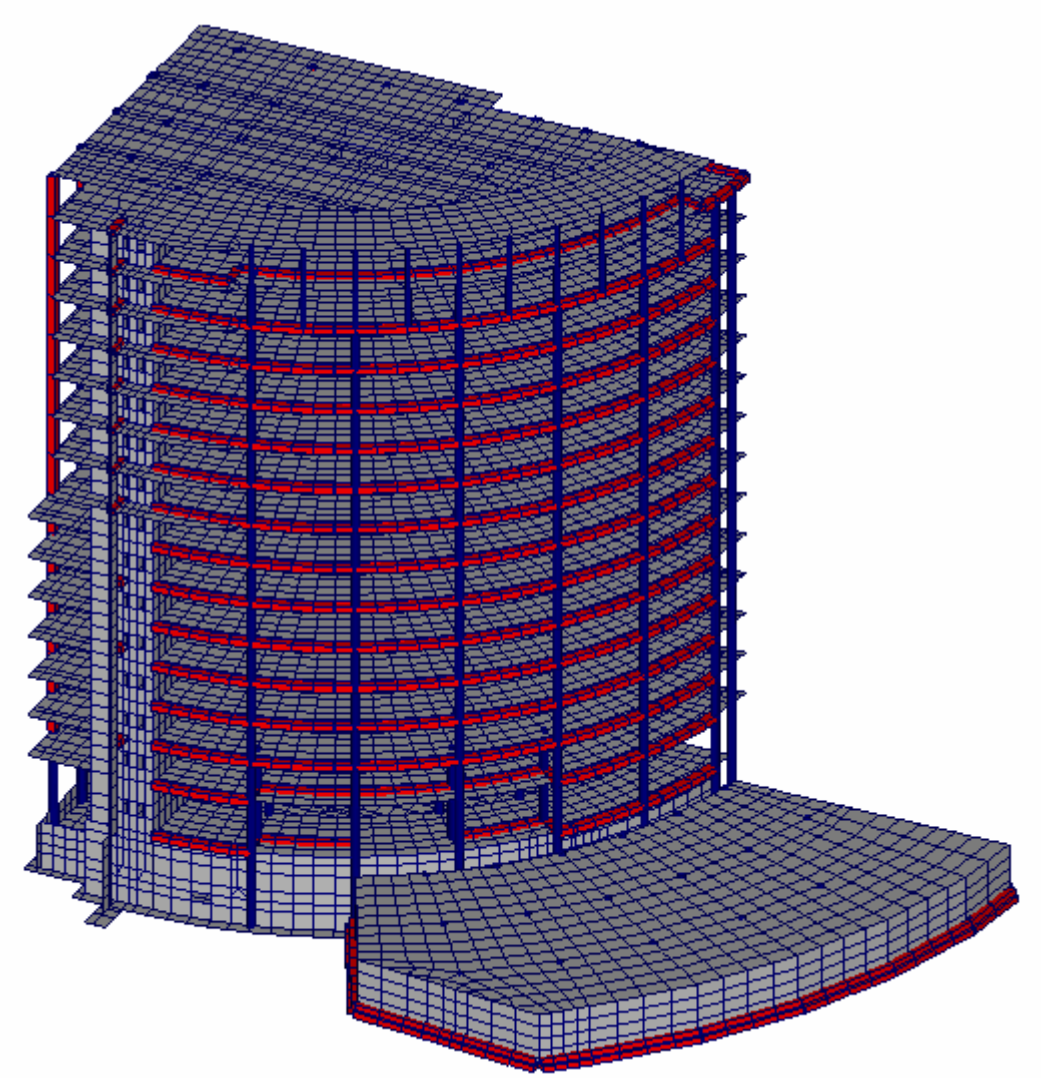

Fig. 6. A multi-storey building (24 434 nodes, 26 273 finite elements, 127 165 equations)

The multi-frontal solver informs us of such instability which leads to very small pivots during the Gauss elimination. But the modes of instability (mechanism modes) have been detected only in the verification mode of the BLST method. Moreover, the verification mode allows us to detect unconstrained bottoms of columns too (Fig. 8).

References

[1] Clough, R. and Penzien, J., *Dynamics of structures*, McGraw-Hill, Inc., 1975.

[2] Ericsson, T. Ruhe, A., The spectral transformation Lanczos method for the numerical solution of large sparse generalize symmetric eigenvalue problem, *Math. Comput.,* 35, pp. 1251-1268, 1980.

[3] Fialko, S.Yu., High-performance iterative and sparse direct solvers in Robot software for static and dynamic analysis of large-scale structures. *Proceedings of the second European conference on computational mechanics*, Poland, June 26-29, 2001, 18 p.

[4] Grimes, R.G. Lewis, J.G., Simon, H.D., A shifted block Lanczos algorithm for solving sparse symmetric generalized eigenproblems, *SIAM J. Matrix Anal. Appl,* V.15, 1: pp. 1-45, 1994.

[5] Hughes, T.J.R., *The finite element method*, Prentice Hall, Englewood Cliffs, NJ, 1987

[6] Parlett, B., *The symmetric eigenvalue problem*, Prentice-Hall, Englewood Cliffs, NJ, 1980.

[7] Papadrakakis, M., *Solving large –scale problems in mechanics*, John Wiley & Sons Ltd., 1993.

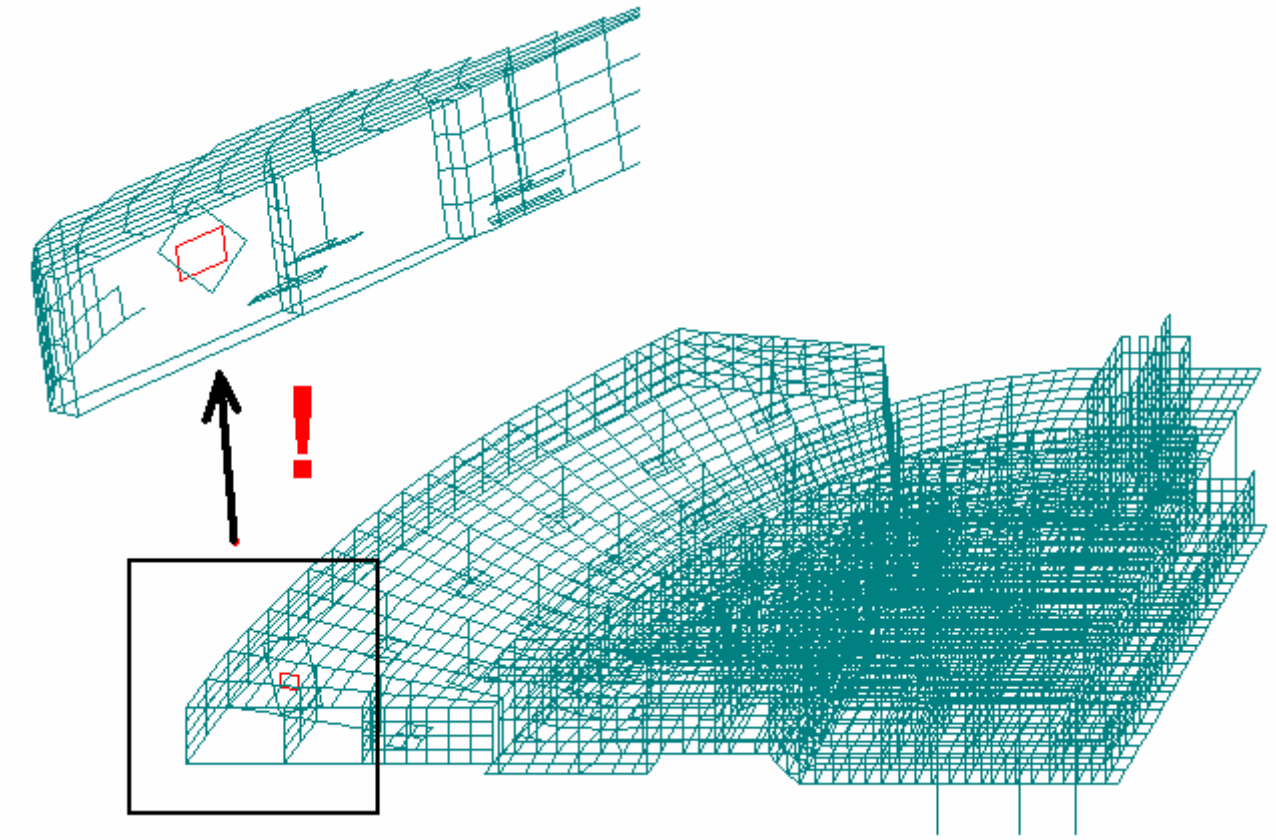

Fig.7 An unconstrained part of structure is detected

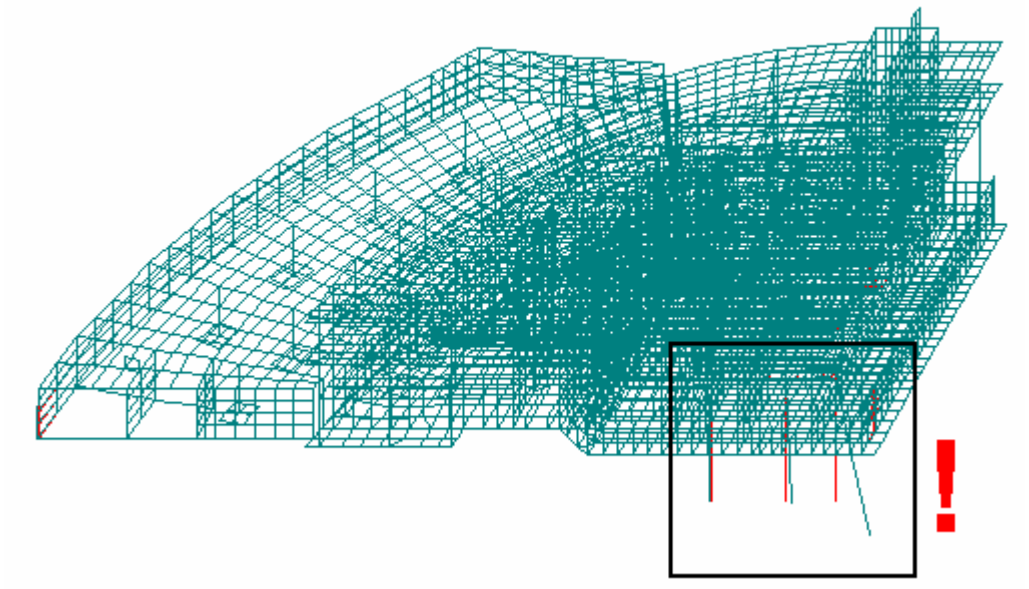

Fig.8 Unconstrained bottoms of columns are detected

[8] Simon, H., *The Lanczos algorithm with partial reorthogonalization*, Math. Comp., 42, pp. 115-136, 1984.

[9] Wilson, E.L., *Three dimensional dynamic analysis of structures*, Computers and Structures, Inc., Berkeley, California, USA, 1996.