

DESIGN OF PARALLEL BLOCK LANCZOS CODE BASED ON DATA STRUCTURE OF MULTIFRONTAL SOLVER

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ABSTRACT

We discuss the assigning scheme of the Lanczos vectors for distributed-memory parallel architectures with the MPI protocol. The eigenvalue problem investigated belongs to the symmetric generalized one with the mass matrix which results from the finite element method. The distributing idea of the Lanczos vectors is developed from the data structure of the multifrontal linear solver. Each processor stores only its own part of the mass matrix and the Lanczos vectors, and the inner product about the mass matrix is simply computed by one call of collective communication about a scalar. In addition, the solution procedure for a linear equation originated from the generalized eigenvalue problem is started with the Lanczos vectors without modifications or communications. Finally, the performance of the code developed is enhanced by using the level 3 BLAS which can be applied only to the block Lanczos algorithm. Using the code developed with such an idea, the performance and the scalability are tested and compared with commercial codes.

PARALLEL IMPLEMENTATION OF LANCZOS ITERATION

Consider a generalized eigenvalue problem

$$KX = \lambda MX \quad (1)$$

where K and M are symmetric positive semi-definite. The shift-invert scheme is utilized for such a generalized problem. Using a factorized form of M , $M = LL^T$, the original problem can be expressed as

$$\frac{1}{\alpha} L^T X = L^T (K - \sigma M)^{-1} LL^T X \quad (2)$$

, where α is shifted eigenvalue. The M orthogonal property is deduced from the transformed vector $L^T X$. Therefore, the M orthogonal Lanczos iteration for a generalized eigenvalue problem is given by the following procedures.

$$\begin{aligned}
U_j &= MV_j && : \text{step } a \\
(K - \sigma M)W_j &= U_j && : \text{step } b \\
W_j^* &= W_j - V_{j-1}B_{j-1}^T && : \text{step } c \\
C_j &= \langle V_j, W_j^* \rangle && : \text{step } d \\
W_j^{**} &= W_j^* - V_j C_j && : \text{step } e \\
W_j^{**} &= V_{j+1}B_j \quad (QR \text{ factorization})
\end{aligned}$$

Figure 1. M orthogonal Lanczos iteration

In Figure 1, $\langle \cdot, \cdot \rangle$ denotes the inner product about M . For a block Lanczos iteration, the basis V_j is a blocked one orthogonalized within itself as $\langle V_j, V_j \rangle = I$. The total amount of computation stems from *step b*, but since it is dependent on the linear equation solver, we do not discuss *step b* in detail. Considering the remaining steps, the distribution of V_j through the processors involved is most important in the parallel version of the Lanczos iteration. In the present research, the distributing scheme is based on the data structure of multifrontal solver. Each processor has its own part $X_{p,f}$ or $X_{p,p}$ of vector X and the inner product about M is obtained by the following relation.

$$\begin{aligned}
Y_{p,p}' &= M_{p,p} Y_{p,f} \\
X_{p,f}^T Y_{p,p}' &= \langle X_{p,f}, Y_{p,f} \rangle \\
\sum_{n=1}^{np} \langle X_{p,f}, Y_{p,f} \rangle &= \langle X, Y \rangle
\end{aligned} \tag{3}$$

, by which the inner product can be computed by only a collective communication about a scalar $\langle X_{p,f}, Y_{p,f} \rangle$. In addition, with such a multiplication of matrix M and vector X , *step b* can be directly followed by *step a*.

In the final presentation, the performance of the vector distributing scheme is shown from the point of view of scalability and some comparison with commercial FEM softwares is also presented.