Stable computations of generalized inverses of positive semidefinite matrices

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Summary. Effective implementation of some efficient FETI methods assumes application of a direct method for solving a system of linear equations with a symmetric positive semidefinite matrix $\mathbf{A}$. The latter usually comprises a triangular decomposition of a nonsingular diagonal block $\mathbf{A}_{JJ}$ of the stiffness matrix $\mathbf{A}$ of a subdomain and an effective evaluation of the action of a generalized inverse of the corresponding Schur complement. The other posibility consists in a regularization of $\mathbf{A}$ resulting in a non-singular matrix $\mathbf{A}_\rho$ whose (standard) inverse is the generalized inverse to $\mathbf{A}$. It avoids the necessity to identify zero pivots with negligible fill-in. We review both these techniques.

1 Introduction

Due to the rounding errors, effective elimination of the displacements of "floating" subdomains is a nontrivial ingredient of implementation of FETI methods, as it can be difficult to recognize the positions of zero pivots when the nonsingular diagonal block of $\mathbf{A}$ is ill-conditioned. Moreover, even if the zero pivots are recognized properly, it turns out that the ill-conditioning of the nonsingular submatrix defined by the nonzero pivots can have a devastating effect on the precision of the solution.

Most of the results are related to the first problem, i.e., to identify reliably the zero pivots. Thus [6] proposed to combine the Cholesky decomposition with the singular value decomposition (SVD) of the related Schur complement $\mathbf{S}$ in order to guarantee a proper rank of the generalized inverse. A natural modification of their method is to carry out the Cholesky decomposition as long as sufficiently large pivots are generated, and then to switch to SVD of $\mathbf{S}$. The dimension of $\mathbf{S}$ is typically small, not greater than four for 2D problems or $3m+3$ for 3D problems of linear elasticity, where m is the number of the last nodes that can be placed on a line.

Here we review our results [2, 5] related to the solution of SPS systems arising in FETI methods. In particular in the Total FETI, a variant [4] of the FETI domain decomposition method that implements both prescribed displacements and interface conditions by the Lagrange multipliers, so that the kernels of the stiffness matrices of

the subdomains, i.e., their rigid body motions, are known a priori. We show, using a suitable (left) generalized inverse, how to reduce the solution of local SPS systems to the decomposition of an a priori defined well-conditioned positive definite diagonal block $\mathbf{A}_{JJ}$ of $\mathbf{A}$ and application of a suitable generalized inverse of its Schur complement $\mathbf{S}$. Since the Schur complement $\mathbf{S}$ in our approach is typically very small, the generalized inverse can be effectively evaluated by the SVD. If the rank of $\mathbf{A}$ or a lower bound on the nonzero eigenvalues of $\mathbf{A}$ are known, as happens in the implementation of TFETI, then the SVD can be implemented without any "epsilon". Moreover, if the kernel of $\mathbf{A}$ is known, then the SVD decomposition can be replaced by effective regularization. Alternatively, we show ([5]) that the kernel can be used to identify a reasonably conditioned nonsingular submatrix of $\mathbf{A}$ of the maximal order, so that $\mathbf{S} = \mathbf{O}$. Our method can be considered as a variant of the regularization method or the LU–SVD method of [6] with a priori choice of the well-conditioned nonsingular part of $\mathbf{A}$ based on a combination of mechanical and combinatorial arguments. Related methods which use an information from the kernel to determine the positions of zero pivots were also proposed by [11, 1].

We review also results of [9], where we proposed a regularization technique enabling us to define a non-singular matrix $\mathbf{A}_\rho$ whose inverse is the generalized inverse to $\mathbf{A}$. It avoids the necessity to identify zero pivots. The favorable feature of our regularization is that an extra fill-in effect in the pattern of the matrix may be negligible.

2 Cholesky decomposition and fixing nodes

We assume that $\mathbf{A}$ is an SPS stiffness matrix of a "floating" 2D or 3D elastic body, such as a subdomain in the TFETI method. If we choose M of the total N mesh nodes that are neither near each other nor placed near any line, $M < N$, $M \geq 2$ in 2D, and $M \geq 3$ in 3D, then the submatrix $\mathbf{A}_{JJ}$ of the stiffness matrix $\mathbf{A}$ defined by the set J with the indices of the displacements of the other nodes is "reasonably" nonsingular. This is not surprising, as $\mathbf{A}_{JJ}$ can be considered as the stiffness matrix of the body that is fixed in the chosen nodes. It is natural to assume that if fixing of the chosen nodes makes the body stiff, then $\mathbf{A}_{JJ}$ is well-conditioned. We call the M chosen nodes *fixing nodes* and denote by I the set of indices of corresponding displacements. In this section, we show how to combine this observation with the regularization of the Schur complement ([12]) or with the LU–SVD method proposed by [6].

Our starting point is the following decomposition of the SPS matrix $\mathbf{A} \in \mathbb{R}^{n \times n}$

$$\widetilde{\mathbf{A}} = \mathbf{P}\mathbf{A}\mathbf{P}^T = \begin{bmatrix} \widetilde{\mathbf{A}}_{JJ} & \widetilde{\mathbf{A}}_{JI} \\ \widetilde{\mathbf{A}}_{IJ} & \widetilde{\mathbf{A}}_{II} \end{bmatrix} = \begin{bmatrix} \mathbf{L}_{JJ} & \mathbf{O} \\ \mathbf{L}_{IJ} & \mathbf{I} \end{bmatrix} \begin{bmatrix} \mathbf{L}_{JJ}^T & \mathbf{L}_{IJ}^T \\ \mathbf{O} & \mathbf{S} \end{bmatrix}, \tag{1}$$

where $\mathbf{L}_{JJ} \in \mathbb{R}^{r \times r}$ is a lower factor of the Cholesky decomposition of $\widetilde{\mathbf{A}}_{JJ}$, $\mathbf{L}_{IJ} \in \mathbb{R}^{s \times r}$, $r = n - s$, $s = 2M$ in 2D, $s = 3M$ in 3D, $\mathbf{L}_{IJ} = \widetilde{\mathbf{A}}_{IJ}\mathbf{L}_{JJ}^{-T}$, $\mathbf{P}$ is a permutation matrix, and $\mathbf{S} \in \mathbb{R}^{s \times s}$ is the Schur complement matrix defined by

$$\mathbf{S} = \widetilde{\mathbf{A}}_{II} - \widetilde{\mathbf{A}}_{IJ}\widetilde{\mathbf{A}}_{JJ}^{-1}\widetilde{\mathbf{A}}_{JI}.$$

To find $\mathbf{P}$, we proceed in two steps. First we form a permutation matrix $\mathbf{P}_1$ to decompose $\mathbf{A}$ into blocks

$$\mathbf{P}_1 \mathbf{A} \mathbf{P}_1^T = \begin{bmatrix} \mathbf{A}_{JJ} & \mathbf{A}_{JI} \\ \mathbf{A}_{IJ} & \mathbf{A}_{II} \end{bmatrix}, \tag{2}$$

where the submatrix $\mathbf{A}_{JJ}$ is nonsingular and $\mathbf{A}_{II}$ corresponds to the degrees of freedom of the M fixing nodes. Then we apply a suitable reordering algorithm on $\mathbf{P}_1 \mathbf{A} \mathbf{P}_1^T$ to get a permutation matrix $\mathbf{P}_2$ which leaves the part $\mathbf{A}_{II}$ without changes and enables the sparse Cholesky decomposition of $\mathbf{A}_{JJ}$. Further, we decompose $\mathbf{P} \mathbf{A} \mathbf{P}^T$ as shown in (1) with $\mathbf{P} = \mathbf{P}_2 \mathbf{P}_1$. To preserve sparsity we use any sparse reordering algorithm such as symmetric approximate minimum degree, symmetric reverse Cuthill-McKee, profile and wavefront reduction etc. The choice depends on the way in which the sparse matrix is stored and on the problem geometry. It is easy to verify that

$$\mathbf{A}^+ = \mathbf{P}^T \begin{bmatrix} \mathbf{L}_{JJ}^{-T} & -\mathbf{L}_{JJ}^{-T} \mathbf{L}_{IJ}^T \mathbf{S}^+ \\ \mathbf{O} & \mathbf{S}^+ \end{bmatrix} \begin{bmatrix} \mathbf{L}_{JJ}^{-1} & \mathbf{O} \\ -\mathbf{L}_{IJ} \mathbf{L}_{JJ}^{-1} & \mathbf{I} \end{bmatrix} \mathbf{P}, \tag{3}$$

where $\mathbf{S}^+ \in \mathbb{R}^{s \times s}$ denotes a left generalized inverse which satisfies

$$\mathbf{S} = \mathbf{S} \mathbf{S}^+ \mathbf{S}.$$

Since s is small, we can substitute for $\mathbf{S}^+$ the Moore–Penrose generalized inverse $\mathbf{S}^\dagger \in \mathbb{R}^{s \times s}$ computed by the SVD. To see that $\mathbf{S}^\dagger$ can be evaluated effectively, first observe that the eigenvectors of $\mathbf{S}$ that correspond to the zero eigenvalues are the traces of the vectors from the kernel of $\mathbf{A}$ on the fixing nodes. Indeed, if $\widetilde{\mathbf{A}} \mathbf{e} = \mathbf{o}$, then

$$\widetilde{\mathbf{A}}_{JJ} \mathbf{e}_J + \widetilde{\mathbf{A}}_{JI} \mathbf{e}_I = \mathbf{o}, \qquad \widetilde{\mathbf{A}}_{IJ} \mathbf{e}_J + \widetilde{\mathbf{A}}_{II} \mathbf{e}_I = \mathbf{o},$$

and

$$\mathbf{S} \mathbf{e}_I = (\widetilde{\mathbf{A}}_{II} - \widetilde{\mathbf{A}}_{IJ} \widetilde{\mathbf{A}}_{JJ}^{-1} \widetilde{\mathbf{A}}_{JI}) \mathbf{e}_I = \widetilde{\mathbf{A}}_{II} \mathbf{e}_I - \widetilde{\mathbf{A}}_{IJ} \widetilde{\mathbf{A}}_{JJ}^{-1} (-\widetilde{\mathbf{A}}_{JJ} \mathbf{e}_J) = \mathbf{o}. \tag{4}$$

Thus if we know the defect d of $\mathbf{A}$, which is the case in the problems arising from application of the TFETI method, we can replace d smallest nonzero eigenvalues of $\mathbf{S}$ by zeros to get the best approximation of $\mathbf{S}$ with the correct rank $s - d$. Alternatively, we can identify the zero eigenvalues correctly if we know a lower bound c on the smallest nonzero eigenvalues of $\mathbf{A}$. Due to the Schur complement eigenvalue interlacing property proved by [13], it follows that the nonzero eigenvalues of $\mathbf{S}$ are also greater or equal to c, so we can replace the computed eigenvalues of $\mathbf{S}$ that do not exceed c by zeros to get an approximation of $\mathbf{S}$ that complies with our information on $\mathbf{A}$. If neither is the case, it seems that the best we can do is to choose some small ε and to replace the eigenvalues that are smaller than ε by zeros (see, e.g., [6, 11]).

It follows from (4) that the kernel of $\mathbf{S}$ is spanned by the trace of a basis of the kernel of $\mathbf{A}$ on the fixing nodes. Assume that the kernel of $\mathbf{A}$ is known, i.e., we know $\mathbf{R} \in \mathbb{R}^{n \times d}$ whose columns span the kernel of $\mathbf{A}$. Assembling $\mathbf{R}_{I*}$ by Ith rows of $\mathbf{R}$, we define the orthogonal projector onto the kernel of $\mathbf{S}$ by

$$\mathbf{Q} = \mathbf{R}_{I*} \left(\mathbf{R}_{I*}^T \mathbf{R}_{I*} \right)^{-1} \mathbf{R}_{I*}^T$$

and we replace $\mathbf{S}^+$ in (3) by

$$\mathbf{S}^* = (\mathbf{S} + \rho \mathbf{Q})^{-1} = \mathbf{S}^\dagger + \rho^{-1} \mathbf{Q}, \quad \rho > 0.$$

We use $\rho \approx \|\mathbf{A}\|$. To see that $\mathbf{S}^*$ is a left generalized inverse, notice that

$$\mathbf{S}\mathbf{S}^*\mathbf{S} = \mathbf{S}(\mathbf{S}+\rho\mathbf{Q})^{-1}\mathbf{S} = \mathbf{S}\left(\mathbf{S}^\dagger + \rho^{-1}\mathbf{Q}\right)\mathbf{S} = \mathbf{S}\mathbf{S}^\dagger\mathbf{S} + \rho^{-1}\mathbf{S}\mathbf{Q}\mathbf{S} = \mathbf{S}.$$

Such approach can be considered as a variant of regularization by [12]. In the next section, we show how to carry out the regularization directly on $\mathbf{A}$.

3 Regularization

This section deals with generalized inverses, for which the necessity to recognize zero pivots is avoided. We regularize $\mathbf{A} \in \mathbb{R}^{n \times n}$ using the known matrix $\mathbf{R} \in \mathbb{R}^{n \times d}$ whose columns span the kernel of $\mathbf{A}$. Although our regularization is general, i.e., it works for rectangular matrices (see [9]), we confine ourself to the SPS matrix $\mathbf{A}$.

Let us introduce the matrix $\mathbf{M} \in \mathbb{R}^{n \times d}$ so that $\mathbf{M}^\top \mathbf{R}$ is nonsingular. Let us assemble to $\mathbf{A}$ the regularized matrix $\mathbf{A}_\rho$ as follows:

$$\mathbf{A}_\rho = \mathbf{A} + \rho \mathbf{M}\mathbf{M}^\top, \tag{5}$$

where $\rho > 0$ is fixed. The following results are proved in [9].

Theorem 1. *The matrix* $\mathbf{A}_\rho$ *is symmetric, positive definite (and non-singular) and its inverse* $\mathbf{A}_\rho^{-1}$ *is the generalized inverse to* $\mathbf{A}$.

Remark 1. If $\mathbf{M} = \mathbf{R}$, we can get the Moore-Penrose inverse $\mathbf{A}^\dagger$ to $\mathbf{A}$ by

$$\mathbf{A}^\dagger = \mathbf{A}_\rho^{-1} \mathbf{P}_{ImA}, \tag{6}$$

where $\mathbf{P}_{ImA} = \mathbf{I} - \mathbf{R}(\mathbf{R}^\top \mathbf{R})^{-1}\mathbf{R}$ is the orthogonal projector on the image of $\mathbf{A}$.

Remark 2. If $\mathbf{A}^+$ is an arbitrary generalized inverse to $\mathbf{A}$, then the Moore-Penrose inverse $\mathbf{A}^\dagger$ is given by

$$\mathbf{A}^\dagger = \mathbf{P}_{ImA}\mathbf{A}^+\mathbf{P}_{ImA} \tag{7}$$

where $\mathbf{P}_{ImA}$ is the same as in Remark 1.

Using (7), one can prove that FETI type algorithms are invariant to the choice of generalized inverses in the sense that each generalized inverse is internally adapted to the Moore-Penrose one [9]. On the other hand, the Moore-Penrose inverse may be directly used in computations via the formulas (6) and (7). Although it should not

affect the behavior of the FETI algorithm, it may stabilize computations for numerically unstable problems; see [10] for the experimental example.

Let us return to computational aspects of the regularization (5). To construct the regularization term, we use again fixing nodes, in which we fix only some DOFs to keep the sparsity pattern of $\mathbf{A}$ in $\mathbf{A}_\rho$ as small as possible (see Fig. 1). Let us denote the set of indices of the fixing DOFs by I and the set of remaining indices by J. We assemble $\mathbf{M}$ as follows:

$$\mathbf{M} = \widetilde{\mathbf{M}}\mathbf{T}, \quad \widetilde{\mathbf{M}}_{i,:} = \left\langle \begin{matrix} \mathbf{R}_{i,:}, \ i \in I, \\ 0, \ i \in J, \end{matrix} \right., i = 1,\ldots,k, \tag{8}$$

where $\mathbf{R}_{i,:}$ denotes the ith row of $\mathbf{R}$ and $\mathbf{T}$ is a nonsingular matrix which orthonormalizes columns of $\widetilde{\mathbf{M}}$ to protect the condition number of $\mathbf{A}_\rho$. Obviously, $\mathbf{T}$ can be efficiently computed as the upper triangular factor of the Cholesky decomposition of $\widetilde{\mathbf{M}}^\top\widetilde{\mathbf{M}}$. Finally, ρ is chosen as the maximum diagonal entry of $\mathbf{A}$ that lays between the minimum and maximum nonzero eigenvalues of $\mathbf{A}$.

The factorization $\mathbf{A}_\rho = \mathbf{L}\mathbf{L}^\top$ can be computed by the Cholesky algorithm for nonsingular matrices. The inverse $\mathbf{A}_\rho^{-1}$ (and the generalized inverse) is given by $\mathbf{A}_\rho^{-1} = \mathbf{L}^{-\top}\mathbf{L}^{-1}$. The computational complexity for band matrices is analyzed in [9]. For the sparse matrices we use a sparse Cholesky factorization in the form $\mathbf{A}_\rho = \mathbf{P}\mathbf{L}\mathbf{L}^\top\mathbf{P}^\top$, where $\mathbf{P}$ is the permutation matrix minimizing fill-in using a suitable reordering algorithm. The action of $\mathbf{A}_\rho^{-1}$ on a vector $\mathbf{v}$ is implemented as follows: $\mathbf{A}_\rho^{-1}\mathbf{v} = \mathbf{P}(\mathbf{L}^{-\top}(\mathbf{L}^{-1}(\mathbf{P}^\top\mathbf{v})))$, where the actions of $\mathbf{L}^{-\top}$ and $\mathbf{L}^{-1}$ are evaluated efficiently using backward and forward substitutions, respectively.

4 Choice of fixing nodes

To get M uniformly distributed fixing nodes we combine a mesh partitioning algorithm with a method for finding mesh centers. The algorithm reads as follows.

ALGORITHM ([2]) Given a mesh and $M > 0$.

1. Split the mesh into M submeshes using the mesh partitioning algorithm.
2. Verify whether the resulting submeshes are connected. If not, a graph postprocessing may be used to get connected submeshes.
3. Take a node lying near the center of each submesh.

Step 1 can be carried out by a code for graph decompositions such as METIS, while Step 3 can be efficiently performed using the so-called Perron vector (a unique nonnegative eigenvector corresponding to the largest eigenvalue of the mesh adjacency matrix) whose maximal entry enables us to approximate the center of the submesh. For more details see [2].

The number of DOFs given by M fixing nodes may be larger than the dimension of the kernel of $\mathbf{A}$. It is useful for engineering problems with complicated geometry. The usage of $\mathbf{M}$ instead of $\mathbf{R}$ in the regularization technique of Section 3 enables us to analyse cases when the most rows of $\mathbf{R}$ are replaced by zeros in $\mathbf{M}$. Then the regularization term in $\mathbf{A}_\rho$ influeces only few entries of $\mathbf{A}$.

5 Cholesky decomposition and the kernel of A

If the kernel of $\mathbf{A}$ is known, then we can use it to identify a submatrix $\mathbf{A}_{JJ}$ of $\mathbf{A}$ of a maximal order. Since the Schur complement of $\mathbf{A}_{JJ}$ is the zero matrix, the solution of a consistent system with $\mathbf{A}$ reduces to the Cholesky decomposition of $\mathbf{A}_{JJ}$. The following estimate proved in [5] indicates that we can use information obtained from the kernel of $\mathbf{A}$ to identify suitable zero pivots.

Proposition 1. *Let $\mathbf{A} \in \mathbb{R}^{n \times n}$ denote a symmetric matrix whose kernel is spanned by the full column rank matrix $\mathbf{R} \in \mathbb{R}^{n \times d}$ with orthonormal columns, so that d is the defect of $\mathbf{A}$. Let $I = \{i_1, \ldots, i_d\}, \quad 1 \le i_1 < i_2 < \cdots < i_d \le n$, denote a set of indices, and let $J = \mathcal{N} - I, \quad \mathcal{N} = \{1, 2, \ldots, n\}$. Then*

$$\lambda_{\min}(\mathbf{A}_{JJ}) \ge \overline{\lambda}_{\min}(\mathbf{A})\, \sigma^4_{\min}(\mathbf{R}_{I*}), \tag{9}$$

where $\overline{\lambda}_{\min}(\mathbf{A})$ and $\sigma_{\min}(\mathbf{R}_{I*})$ denote the least nonzero eigenvalue of $\mathbf{A}$ and the least singular value of $\mathbf{R}_{I*}$.

This strategy chooses d fixing DOFs by the orthonormalization of $\mathbf{R}$ and applying the Gaussian elimination with complete pivoting to transform orthonormalized matrix $\mathbf{R}$ into the column-wise echelon form. The position of the first nonzero entry in each column gives the degree of freedom which will be fixed. For more details we refer to [5].

6 Numerical examples

The performance of our strategies is tested on the stiffness matrix $\mathbf{A}$ of the elastic three-dimensional cube made of steel and discretized by trilinear bricks with the Neumann boundary conditions (see Fig. 1.(a)). To illustrate the effect of fixing nodes,
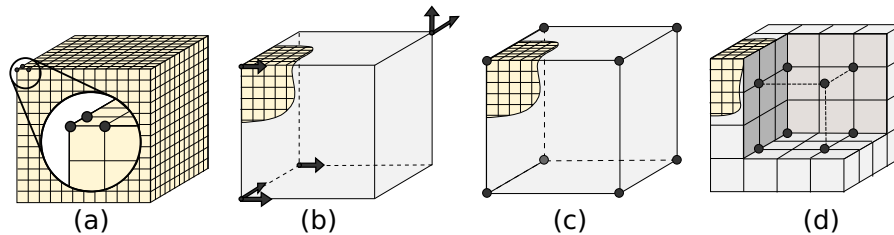
Fig. 1. (a) No strategy, (b) GP strategy, (c) Geometrical strategy, (d) Uniform strategy

we carried out the computations for different strategies of choosing fixing nodes depicted in Fig. 1. Here *Geometrical strategy* is the simplest one and is based on finding fixing nodes using simple geometrical and combinatorial arguments: choose

M mesh nodes that are mutually as far apart as possible and that are not placed near any line.

In Table 1, we report the regular condition number $\overline{\text{cond}}(\mathbf{A})$ (ratio of the largest and the smallest nonzero eigenvalues), the condition number of the nonsingular part $\mathbf{A}_{JJ}$ decomposed by the Cholesky decomposition, and the regular condition number $\overline{\text{cond}}(\mathbf{A}^+)$. The results of experiments agree with the intuitive rule that fixing nodes distributed in a more regular pattern improves the conditioning of $\mathbf{A}_{JJ}$. In particular, comparing variants (c) and (d), we can observe that placing the eight fixing nodes inside the body can result in more stable generalized inverse than placing them at the corners. It follows that the matrices arising in the original FETI method or its TFETI variant are typically better conditioned than those arising in the FETI–DP. Notice that the worst conditioning of $\mathbf{A}_{JJ}$ and $\mathbf{A}^+$ can be observed in variant (a) which is a possible result of the default strategy used by Farhat and Géradin [6].

Table 1. Characteristics of $\mathbf{A}$ and $\mathbf{A}^+$ in dependence on the distribution of fixing nodes.

	No strategy	GP strategy	Geometrical strategy	Uniform strategy
$\overline{\text{cond}}(\mathbf{A})$	4.91E+02	4.91E+02	4.91E+02	4.91E+02
$\text{cond}(\mathbf{A}_{JJ})$	2.90E+07	3.52E+05	9.92E+03	1.90E+03
$\overline{\text{cond}}(\mathbf{A}^+)$	2.55E+07	3.52E+05	1.32E+04	1.90E+03

Table 2 shows results of numerical tests based on the regularization. The rows *iter* or *iter*† report iterations of the TFETI algorithm for the regularizations computed by strategies (b)-(d) or by the Moore-Penrose inverse obtained from them using (7), respectively. It confirms invariancy with respect to the choice of the generalized inverse. The condition numbers in the next two rows agree with the same heuristic as in Table 1, i.e., the conditioning of A_ρ^{-1} is improved when the fixing DOFs are distributed in a more regular pattern. The CPU times in the fifth and sixth rows required for computing the Cholesky decomposition and the actions of the generalized inverses, respectively, illustrate the computational invariancy that is due to the negligible fill-in. It is seen from the number of non-zero entries in the last row of the table.

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Table 2. Characteristics of $\mathbf{A}$ and $\mathbf{A}_\rho^{-1}$ in dependence on the distribution of fixing nodes.

	GP strategy	Geometrical strategy	Uniform strategy
iter	22	22	22
iter†	22	22	22
$\overline{\text{cond}}(\mathbf{A})$	4.91E+02	4.91E+02	4.91E+02
cond($\mathbf{A}_\rho^{-1}$)	3.53e+05	1.30e+04	3.02e+03
chol [sec.]	0.2897	0.2750	0.2567
action [sec.]	0.0215	0.0209	0.0210
nnz_chol	2775956	2762089	2690104

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