

## Accelerated Simultaneous Iterations for Large Finite Element Eigenproblems

FLAVIO SARTORETTO, GIORGIO PINI, AND GIUSEPPE GAMBOLATI

*Università di Padova, Istituto di Matematica Applicata,  
Via Belzoni, 7, 35131 Padua, Italy*

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An accelerated simultaneous iteration method is presented for the solution of the generalized eigenproblem  $\mathbf{Ax} = \lambda\mathbf{Bx}$ , where  $\mathbf{A}$  and  $\mathbf{B}$  are real sparse symmetric positive definite matrices. The approach is well suited for the determination of the leftmost eigenpairs of problems with large size  $N$ . The procedure relies on the optimization of the Rayleigh quotient over a subspace of orthogonal vectors by a conjugate gradient technique effectively preconditioned with the pointwise incomplete Cholesky factorization. The method is applied to the evaluation of the smallest 15 eigenpairs of finite element models with size ranging between 150 and 2300. The numerical experiments show that, while the simultaneous conjugate gradient scheme fails to converge, the accelerated iterations yield accurate results in a number of steps which is much smaller than  $N$ . The new approach does not require the a priori estimate of any empirical parameter and appears to be a robust, reliable, and efficient tool for the partial eigensolution of large finite element problems. © 1989 Academic Press, Inc.

### INTRODUCTION

The evaluation of the  $p$  leftmost eigenpairs of the generalized eigenvalue problem

$$\mathbf{Ax} = \lambda\mathbf{Bx},$$

where  $\mathbf{A}$  and  $\mathbf{B}$  are large sparse symmetric positive definite matrices, is an important task in many engineering and physical problems, e.g., in structural mechanics [1–3], hydrodynamics [4] and plasma physics [5–7]. Typically the value of  $p$  is much smaller than the matrix size  $N$ , which may be several hundreds or even many thousands large.

To find the eigensolution of sparse linear problems the Lanczos method [8] has been used (Paige [9]; Cullum and Willoughby [10, 11]). A block generalization, especially designed for the extreme eigenpairs of  $\mathbf{A}$ , has been developed by Golub and Underwood [12] and Cullum and Donath [13]. The Lanczos method and its variants require several iterations (sometimes more than  $N$ ) to converge to an accurate approximation of the leftmost eigenspectrum. Spectral transformations employing the Lanczos technique have been proposed by Ericsson and Ruhe [14],

but they require the triangular factorization of several shifted matrices. Although attractive at the theoretical level, this approach is precluded for large arbitrarily sparse matrices on the grounds of impracticality.

Recently iterative algorithms based on multiple Rayleigh quotient optimization [15, 16] or trace minimization [17] or penalty function optimization [18] have been developed. The schemes which rely on the Rayleigh quotient optimization are particularly attractive, since they are simple to implement and well suited to vectorization (for a short review of these methods see [19]). Some of them require the "a priori" knowledge of an empirical acceleration parameter (e.g., the coordinate relaxation method [16, 20]), which reduces drastically their importance in practical applications. Others are based upon the gradient or conjugate gradient (CG) iterations but generally their convergence is very slow with large matrices of arbitrary structure. However the latter may be greatly improved if the CG scheme is effectively preconditioned [21].

An excellent review of several preconditioning techniques may be found in Concus *et al.* [22]. Many preconditioners belong to the class of the incomplete Cholesky decompositions (Evans [23]; Tuff and Jennings, [24]; Concus *et al.* [25]; Axelsson [26]; Jennings and Malik [27]; Gustafsson [28]; Kershaw [29]; Gambolati [30, 31]; Gambolati and Volpi [32]; Gustafsson [33]; Manteuffel [34]; Eisenstat [35]; Appleyard and Cheshire [36]; Axelsson and Gustafsson [37]; Jacobs [38]; Jennings [39]; Ajiz and Jennings [40]; Nour-Omid [41]; Jackson and Robinson [42]; Tismenetsky and Efrat [43]; Wong *et al.* [44]; Zyvoloski [45]). Although sophisticated polynomial [46, 47] and multistep [48] preconditioners have been developed, mainly for the efficient implementation of parallel algorithms, the diagonal scaling and the pointwise incomplete Cholesky factorization of Kershaw [29], referred to as ICCG(0) by Meijerink and van der Vorst [49], represent two of the most inexpensive and widespread choices. In particular ICCG(0) turned out to be a reliable and efficient tool for the solution to both linear systems and eigenproblems in a finite element context (Gambolati *et al.* [50]). Preconditioning has been used along with a stepwise deflation technique [19] to evaluate successfully several of the smallest eigenpairs. The results proved very encouraging and the method rather cost-effective. However, a disadvantage of the approach described in [19] is the need for the assessment of a deflation parameter which is related to the eigenvalues distribution and, although not difficult to estimate in practice, is to some extent problem dependent.

The idea underlying the present work is to accelerate the simultaneous CG methods developed by Longsine and McCormick [15] and Schwarz [16] with the ICCG(0) preconditioning.

It is shown with representative numerical examples, arising from the finite element integration of flow and structural equations, that preconditioning is essential to ensure practical convergence. The new procedure is applied to compute simultaneously the 15 leftmost eigenpairs of arbitrarily sparse matrices whose size ranges from 150 to 2300. The number of iterations required to obtain accurate results turns out to be by far less than  $N$ .

Finally, as was already noted in [15, 16], it is shown that to have a good convergence the overall procedure is to be restarted every 10–20 modified conjugate gradient (MCG) iterations, possibly by performing a Ritz projection step.

### 1. ACCELERATION OF THE SIMULTANEOUS RAYLEIGH QUOTIENT MINIMIZATION

Let  $\mathbf{A}$  and  $\mathbf{B}$  be sparse symmetric positive definite  $N \times N$  matrices. Consider the generalized eigenvalue problem:

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{B}\mathbf{x}. \quad (1)$$

Denote by

$$\lambda_N \leq \lambda_{N-1} \leq \dots \leq \lambda_1$$

and

$$\mathbf{v}_N, \mathbf{v}_{N-1}, \dots, \mathbf{v}_1$$

the eigenvalues and the corresponding eigenvectors.

It can be proved (cf. [51]) that the eigenvectors of (1) are the stationary points of the Rayleigh quotient

$$R(\mathbf{x}) = \frac{\mathbf{x}^T \mathbf{A} \mathbf{x}}{\mathbf{x}^T \mathbf{B} \mathbf{x}} \quad (2)$$

The gradient of  $R(\mathbf{x})$  is given by

$$g(\mathbf{x}) = \frac{2}{\mathbf{x}^T \mathbf{B} \mathbf{x}} (\mathbf{A} \mathbf{x} - R(\mathbf{x}) \mathbf{B} \mathbf{x}). \quad (3)$$

For the sake of brevity we set  $\mathbf{g}^{(k)} = g(\mathbf{x}^{(k)})$ .

Let us consider the Rayleigh quotient conjugate gradient (RQCG) method, which yields the leftmost eigenpair  $(\lambda_N, \mathbf{v}_N)$  of (1), by minimizing (2) along a set of suitable directions (cf. [19]).

Let  $\mathbf{x}^{(0)}$  and  $\mathbf{p}^{(-1)}$  be an initial guessed vector and the zero vector, respectively.

The typical RQCG  $k$ th iteration, with  $k=0, 1, \dots$ , consists essentially of two steps:

- (a) search for a minimization direction  $\mathbf{p}^{(k)}$  expressed as

$$\mathbf{p}^{(k)} = \mathbf{g}^{(k)} + \beta^{(k-1)} \mathbf{p}^{(k-1)}, \quad (4)$$

where  $\beta^{(k-1)}$  is a parameter which will be given later.

(b) evaluation of a new approximation  $\mathbf{x}^{(k+1)}$  to  $\mathbf{v}_N$  along  $\mathbf{p}^{(k)}$  through  $\mathbf{x}^{(k)}$  written as

$$\mathbf{x}^{(k+1)} = \mathbf{x}^{(k)} + \alpha^{(k)}\mathbf{p}^{(k)}, \quad (5)$$

where  $\alpha^{(k)}$  is obtained by minimizing the quantity

$$R(\mathbf{x}^{(k)} + \alpha^{(k)}\mathbf{p}^{(k)}). \quad (6)$$

The RQCG iterations are continued until the relative residual

$$r_r^{(k)} = \frac{\|\mathbf{A}\mathbf{x}^{(k)} - R(\mathbf{x}^{(k)})\mathbf{B}\mathbf{x}^{(k)}\|}{\|\mathbf{A}\mathbf{x}^{(k)}\|}, \quad (7)$$

where  $\|\cdot\|$  stands for the euclidean norm, is smaller than a prescribed tolerance.

Since in most engineering and physical problems it is necessary to compute a number of the leftmost eigenpairs of (1), an extension of the RQCG scheme has been devised [15, 16], which allows for the simultaneous evaluation of the leftmost  $p$  eigenpairs of (1) (in the sequel  $1 \leq p \leq 15$  is assumed).

The basic idea underlying the simultaneous conjugate gradient (SRQCG) iterations is to start from an arbitrary set  $\mathbf{x}_i^{(0)}$ ,  $i = 1, \dots, p$  of vectors and to minimize (2) at the  $k$ th iteration along a set of  $p$  directions  $\mathbf{p}_i^{(k)}$ ,  $i = 1, \dots, p$ .

For the sake of brevity, in the sequel we shall denote by  $\mathbf{x}_i^{(k)}$ ,  $\mathbf{p}_i^{(k)}$ ,  $\mathbf{g}_i^{(k)}$ ,  $k = 1, \dots$ ;  $i = 1, \dots, p$  the columns of the  $N \times p$  matrices  $\mathbf{X}^{(k)}$ ,  $\mathbf{P}^{(k)}$ , and  $\mathbf{G}^{(k)}$ , respectively.

If  $\mathbf{X}^{(k)\top}\mathbf{B}\mathbf{X}^{(k)} = \mathbf{I}_p$ , where  $\mathbf{I}_p$  is the  $p \times p$  identity matrix, we set

$$\mathbf{G}^{(k)} = 2(\mathbf{A}\mathbf{X}^{(k)} - \mathbf{B}\mathbf{X}^{(k)}D_R[\mathbf{X}^{(k)}]); \quad (8)$$

$D_R[\mathbf{X}^{(k)}]$  is the diagonal matrix whose entries are the diagonal coefficients of the  $p \times p$  Rayleigh matrix  $\mathbf{X}^{(k)\top}\mathbf{A}\mathbf{X}^{(k)}$ .

In extending the RQCG algorithm to the evaluation of  $p$  eigenpairs, the minimization parameter  $\alpha^{(k)}$  is substituted by the  $p \times p$  matrix  $\Delta^{(k)}$  such that, as is pointed out in [15], the columns of

$$\mathbf{X}^{(k)} + \mathbf{P}^{(k)}\Delta^{(k)} \quad (9)$$

“in some sense represent the best set of solutions of (1) from  $\text{span}(\mathbf{X}^{(k)}, \mathbf{P}^{(k)})$ , the column span of  $(\mathbf{X}^{(k)}, \mathbf{P}^{(k)})$ .”

In principle,  $\Delta^{(k)}$  is a full  $p \times p$  matrix, but to reduce the computational cost we take into account in (9) only diagonal matrices.

The most natural way to extend the RQCG algorithm is to minimize (6) separately for each search direction. However, to avoid convergence toward the same eigenvector  $\mathbf{v}_N$ , the approximating vectors are to be kept  $\mathbf{B}$ -orthogonal in the iterative procedure.

Note that the vectors  $\mathbf{x}_i^{(k)}$ ,  $i = 1, \dots, p$ , can be thought of as “the (approximated) eigenvectors,” if they converge to  $\mathbf{v}_N, \dots, \mathbf{v}_{N-p+1}$ , when  $k$  increases.

The SRQCG scheme can be described as follows. Let us assume that a set of approximations  $\mathbf{X}^{(k)}$  was computed, together with a set of directions  $\mathbf{P}^{(k)}$  obtained by performing  $p$  times the step (a) of RQCG.

For  $i = 1, \dots, p$ , perform steps 1, 2, 3, 4:

(1) compute  $\tilde{\mathbf{x}}_i^{(k)}$  and  $\tilde{\mathbf{p}}_i^{(k)}$  by  $\mathbf{B}$ -orthogonalizing  $\mathbf{x}_i^{(k)}$  and  $\mathbf{p}_i^{(k)}$  with respect to  $\mathbf{V}_i = \{\mathbf{x}_j^{(k+1)}, j = 1, \dots, i-1\}$ ;

(2) determine the parameter  $\alpha^{(k)}$  which minimizes

$$R(\tilde{\mathbf{x}}_i^{(k)} + \alpha^{(k)}\tilde{\mathbf{p}}_i^{(k)}); \quad (10)$$

(3) compute

$$\tilde{\mathbf{x}}_i^{(k+1)} = \tilde{\mathbf{x}}_i^{(k)} + \alpha^{(k)}\tilde{\mathbf{p}}_i^{(k)}; \quad (11)$$

(4) evaluate  $\mathbf{x}_i^{(k+1)}$  by  $\mathbf{B}$ -normalizing  $\tilde{\mathbf{x}}_i^{(k+1)}$ .

The previous procedure is labelled SIRQCG in [16] and will be called SRQCG1 in the sequel.

A slightly different scheme, named here as SRQCG2 and referred to as SIRQIT-CG by Longsine and McCormick, is proposed in [15]. SRQCG2 consists again of 4 steps, but step 1 does not perform one of the two  $\mathbf{B}$ -orthogonalizations, being  $\tilde{\mathbf{x}}_i^{(k)} = \mathbf{x}_i^{(k)}$ , while in step 4,  $\mathbf{x}_i^{(k+1)}$  is evaluated by  $\mathbf{B}$ -orthonormalizing  $\tilde{\mathbf{x}}_i^{(k+1)}$  with respect to  $\mathbf{V}_i$ .

Let

$$\mathbf{r}_j^{(k)} = \mathbf{A}\mathbf{x}_j^{(k)} - \mathbf{B}\mathbf{x}_j^{(k)}R(\mathbf{x}_j^{(k)}) \quad (12)$$

be the  $j$ th residual vector and  $r_{r_j}^{(k)} = \|\mathbf{r}_j^{(k)}\|/\|\mathbf{A}\mathbf{x}_j^{(k)}\|$  the  $j$ th relative residual.

The SRQCG1 and SRQCG2 schemes repeat the respective iterations until the average relative residual  $r_a^{(k)}$ , defined as

$$r_a^{(k)} = \sqrt{\sum_{j=1}^p (\mathbf{r}_{r_j}^{(k)})^2/p} \quad (13)$$

becomes smaller than a prescribed tolerance TOLL, the leftmost  $p$  eigenpairs being computed, each one with at least a relative accuracy equal to TOLL. The accuracy on the eigenvalues being squared (see [52]), it is also  $\lambda_{N-j+1} = R(\mathbf{x}_j^{(k)})$ ,  $j = 1, \dots, p$ .

Experience shows for SRQMCG1 and SRQMCG2 to converge practically, a recurring "reset" operation is to be executed after a given number NREST of iterations is completed [15, 16].

Such a reset operation might in principle consist of simply restarting the conjugate gradient scheme, namely setting

$$\mathbf{P}^{(k)} = \mathbf{G}^{(k)}, \quad (14)$$

then proceeding from the beginning of the SRQCG iteration. However, the evaluation of a new approximation set  $\mathbf{X}^{(k)}$  through a Ritz projection step proves more

effective, as is shown in the next section. The related “full” restart operation consists of the following operations [16]: first the solution  $\mathbf{Y} = \{\mathbf{y}_i, i = 1, \dots, p\}$  to the problem (1) orthogonally projected over the subspace  $\text{span}(\mathbf{X}^{(k)})$  is derived. The  $\mathbf{y}_i$  are computed in such a way that  $\mathbf{Y}^T \mathbf{B} \mathbf{Y} = \mathbf{I}_p$  and  $\bar{\mathbf{D}} = (\bar{d}_{ij}) = \mathbf{Y}^T \mathbf{A} \mathbf{Y}$  is a diagonal matrix for which if  $i < j$  then  $\bar{d}_{ii} \leq \bar{d}_{jj}$  holds true. Next,  $\mathbf{X}^{(k)} = \mathbf{Y}$  is set and the  $\mathbf{G}^{(k)}$  and  $\mathbf{P}^{(k)}$  directions are obtained from (8) and (14), respectively.

Despite this improvement, SRQCG1 and SRQCG2 prove very inefficient to solve large sparse finite element eigenproblems, as is shown in Section 2.

A similar problem was met in the RQCG computation of the leftmost eigenpair of large sparse matrices [4, 21]. The performance of RQCG was highly enhanced by the use of a suitable preconditioning technique [4, 21], which consists of minimizing the quotient

$$R(\mathbf{y}) = \frac{\mathbf{y}^T \mathbf{X}^{-1} \mathbf{A} \mathbf{X}^{-1} \mathbf{y}}{\mathbf{y}^T \mathbf{X}^{-1} \mathbf{B} \mathbf{X}^{-1} \mathbf{y}}. \quad (15)$$

Equation (15) is derived from (2) by the variables transformation

$$\mathbf{y} = \mathbf{X} \mathbf{x}, \quad (16)$$

$\mathbf{X}$  being a symmetric matrix.

The transformation (16) leaves the stationary values of (2) unchanged, while the corresponding stationary points are readily obtained from (16).

Applying the RQCG scheme to (15), then restoring the original variable  $\mathbf{x}$ , yield the preconditioned scheme [4, 19, 21], where the so-called “preconditioning matrix”

$$\mathbf{K}^{-1} = \mathbf{X}^{-1} \mathbf{X}^{-1}$$

is introduced. Depending upon the choice of  $\mathbf{K}^{-1}$ , a class of preconditioned RQCG procedures is obtained, which we call RQMCG (“M” means modified, i.e., preconditioned).

The combination of a RQMCG algorithm with a deflation technique has led to an efficient scheme for the solution of the partial eigenproblem with  $p$  up to 20. This approach is described in detail in [19]. However, a deficiency of the overall procedure is the need for the a priori assessment of a deflation parameter which, although it is not highly sensitive to the eigenvalues distribution, is problem-dependent. The idea underlying the present work is to precondition the simultaneous iterations SRQCG1 and SRQCG2 (thereafter called SRQMCG1 and SRQMCG2, respectively), thus eliminating the need for any empirical parameter estimate.

We refer to SRQMCG2, which turns out to be slightly more efficient than SRQMCG1. The SRQMCG2 scheme consists of the following steps:

*Step 1.* Define and compute the preconditioning matrix  $\mathbf{K}^{-1}$  (this step will be analysed later).

*Step 2.* Give a  $N \times p$  matrix  $\mathbf{X}^{(0)}$  such that  $\mathbf{X}^{(0)\top} \mathbf{B} \mathbf{X}^{(0)} = \mathbf{I}_p$ , a tolerance value TOLL, the allowed maximum number of iterations NITMAX and a "restart" value NREST. Compute the initial residual matrix as

$$M_r(\mathbf{X}^{(0)}) = \mathbf{A} \mathbf{X}^{(0)} - \mathbf{B} \mathbf{X}^{(0)} D_R(\mathbf{X}^{(0)}) = \frac{1}{2} \mathbf{G}^{(0)} \quad (17)$$

and the average relative residual  $r_a^{(0)}$ . Set  $k = 0$  (iteration index).

As long as  $k$  is smaller than NITMAX and  $r_a^{(k)}$  is greater than TOLL, execute Steps 3, 4, and 5; otherwise go to Step 6.

*Step 3.* If  $\text{mod}(k, \text{NREST}) \neq 0$ ,

3.1.1. Set  $\tilde{\mathbf{X}}^{(k)} = \mathbf{X}^{(k)}$  and evaluate the parameters  $\beta_1, \dots, \beta_p$  by the formula (cf. [53])

$$\beta_j = \frac{\|M_r(\tilde{\mathbf{x}}_j^{(k)})\|_{\mathbf{K}^{-1}}^2}{\|M_r(\tilde{\mathbf{x}}_j^{(k-1)})\|_{\mathbf{K}^{-1}}^2}, \quad (18)$$

where  $\|\mathbf{x}\|_{\mathbf{K}^{-1}}^2 = \mathbf{x}^\top \mathbf{K}^{-1} \mathbf{x}$ .

3.1.2. Set  $\Gamma^{(k-1)} = \text{diag}(\beta_1, \dots, \beta_p)$  and compute

$$\mathbf{P}^{(k)} = \mathbf{K}^{-1} M_r(\tilde{\mathbf{X}}^{(k)}) + \mathbf{P}^{(k-1)} \Gamma^{(k-1)}, \quad (19)$$

otherwise

3.2.1. Compute  $\tilde{\mathbf{X}}^{(k)}$  as the  $\mathbf{B}$ -orthonormal solution to the problem (1) projected onto  $\text{span}(\mathbf{X}^{(k)})$ , the vector subspace generated by the columns of the matrix  $\mathbf{X}^{(k)}$ . This is the Ritz step.

3.2.2. Set

$$\mathbf{P}^{(k)} = \mathbf{K}^{-1} M_r(\tilde{\mathbf{X}}^{(k)}). \quad (20)$$

*Step 4.* Evaluate the new matrix

$$\tilde{\mathbf{X}}^{(k+1)} = \tilde{\mathbf{X}}^{(k)} + \tilde{\mathbf{P}}^{(k)} \Delta^{(k)} \quad \Delta^{(k)} = \text{diag}(\alpha_1, \dots, \alpha_p). \quad (21)$$

More precisely, for each  $j = 1, \dots, p$ :

4.1. The vector  $\tilde{\mathbf{p}}_j^{(k)}$  is evaluated by  $\mathbf{B}$ -orthogonalizing  $\mathbf{p}_j^{(k)}$  with respect to  $\mathbf{V}_j = \{\mathbf{x}_1^{(k+1)}, \dots, \mathbf{x}_{j-1}^{(k+1)}\}$ ;

4.2. The coefficients  $\alpha_j$  are obtained by minimizing the Rayleigh quotient

$$R(\tilde{\mathbf{x}}_j^{(k)} + \alpha_j \tilde{\mathbf{p}}_j^{(k)})$$

and the vector

$$\tilde{\mathbf{x}}_j^{(k+1)} = \tilde{\mathbf{x}}_j^{(k)} + \alpha_j \tilde{\mathbf{p}}_j^{(k)}$$

is computed.

4.3.  $\mathbf{x}_j^{(k+1)}$  is evaluated by  $\mathbf{B}$ -orthonormalizing  $\tilde{\mathbf{x}}_j^{(k+1)}$  with respect to  $\mathbf{V}_j$ .

*Step 5.* Compute the residual matrix  $M_r(\mathbf{X}^{(k+1)})$  together with the value  $r_a^{(k+1)}$ . Increment the iteration counter  $k$  and go back to the loop start.

*Step 6.* If  $r_a^{(k)}$  is smaller than TOLL,  $R(\mathbf{x}_j^{(k)})$  and  $\mathbf{x}_j^{(k)}$ ,  $j=1, \dots, p$ , are the smallest  $p$  eigenvalues of (1) and the corresponding eigenvectors, respectively.

When Step 4.1 is modified by adding the  $\mathbf{B}$ -orthogonalization of  $\tilde{\mathbf{x}}_j^{(k)}$  with respect to  $\mathbf{V}_j$  and the  $\mathbf{B}$ -orthonormalization is substituted by a  $\mathbf{B}$ -normalization in Step 4.3, the variant SRQMCG1 is obtained.

The following remarks are worth emphasizing:

(a) The Ritz step, 3.2.1, is equivalent to solving the problem

$$\mathbf{A}_1 \mathbf{y} = \mu \mathbf{y}, \quad \mathbf{A}_1 = \mathbf{X}^{(k)\top} \mathbf{A} \mathbf{X}^{(k)},$$

where  $\mathbf{y}$  is a  $p$ -dimensional vector and  $\mathbf{X}^{(k)\top} \mathbf{B} \mathbf{X}^{(k)} = \mathbf{I}_p$ . An orthogonal matrix  $\mathbf{Q}$  is found such that

$$\mathbf{Q}^\top \mathbf{A}_1 \mathbf{Q} = \text{diag}(\mu_p, \dots, \mu_1),$$

$\mu_p \leq \dots \leq \mu_1$ ; then we set  $\tilde{\mathbf{X}}^{(k)} = \mathbf{X}^{(k)} \mathbf{Q}$ . So  $\tilde{\mathbf{X}}^{(k)\top} \mathbf{A} \tilde{\mathbf{X}}^{(k)}$  is a diagonal matrix and  $\tilde{\mathbf{X}}^{(k)\top} \mathbf{B} \tilde{\mathbf{X}}^{(k)} = \mathbf{I}_p$ .

(b) The scalars  $\alpha_j$  needed in Step 4.2 are obtained as follows. Set

$$\begin{aligned} \tilde{\mathbf{x}} &= \tilde{\mathbf{x}}_j^{(k)} & \tilde{\mathbf{p}} &= \tilde{\mathbf{p}}_j^{(k)} \\ a &= (\tilde{\mathbf{p}}^\top \mathbf{A} \tilde{\mathbf{x}}) & b &= (\tilde{\mathbf{p}}^\top \mathbf{A} \tilde{\mathbf{p}}) \\ c &= (\tilde{\mathbf{p}}^\top \mathbf{B} \tilde{\mathbf{x}}) & d &= (\tilde{\mathbf{p}}^\top \mathbf{B} \tilde{\mathbf{p}}) \\ m &= (\tilde{\mathbf{x}}^\top \mathbf{B} \tilde{\mathbf{x}}) & n &= (\tilde{\mathbf{x}}^\top \mathbf{A} \tilde{\mathbf{x}}) \end{aligned}$$

$$\delta = (nd - mb)^2 - 4(bc - ad)(ma - nc).$$

It turns out that [19]

$$\alpha_j = \frac{1}{2}(nd - mb + \sqrt{\delta}) / (bc - ad). \quad (22)$$

Consider now the preconditioning matrix  $\mathbf{K}^{-1}$ . For the sake of simplicity we restrict our analysis to the case  $\mathbf{B} = \mathbf{I}_N$ . If  $\mathbf{K}^{-1} = \mathbf{I}_N$ , SRQMCG2 coincides with SRQCG2. The cheapest selection for  $\mathbf{K}^{-1}$  is provided by

$$\mathbf{K}^{-1} = \mathbf{D}^{-1}, \quad (23)$$

$\mathbf{D}$  being the diagonal matrix formed by the diagonal entries of  $\mathbf{A}$ .

However, a more efficient choice in the overall procedure is

$$\mathbf{K}^{-1} = (\mathbf{L}\mathbf{L}^\top)^{-1}, \quad (24)$$

$\mathbf{L}$  being the pointwise incomplete Cholesky factor of  $\mathbf{A}$  [29].

The algorithms SRQMCG2(D) and SRQMCG2(L) are designated accordingly.



## 2. NUMERICAL RESULTS

Some representative numerical results are provided in this section. They were obtained with a FORTRAN code performing double precision operations on the IBM 4341/2 computer of the University of Padua.

Four arbitrarily sparse finite element matrices  $\mathbf{A}$  are considered. They arise from the finite element integration of subsurface 3D flow equations and 2D elasticity equations for layered structures subject to vertical and horizontal land subsidence. The size of  $\mathbf{A}$  is 156, 812, 1802, and 2304. The related irregular sparsity patterns are displayed in [19].

All the figures given in the sequel report the behaviour of the average residual  $r_a^{(k)}$  versus the number of iterations  $k$  in the computation of the leftmost  $p$  eigenpairs.  $\mathbf{B} = \mathbf{I}_N$  and  $p = 15$  is assumed.

The starting set  $\mathbf{X}^{(0)}$  was obtained by orthonormalizing the set of vectors  $\{\mathbf{f}_i, i = 1, \dots, p\}$ , where for each  $i$  and  $j = 1, \dots, N$  we have taken

$$\mathbf{f}_{ij} = \begin{cases} \eta & \text{if } i = j \text{ or } j > p \\ 0 & \text{otherwise,} \end{cases}$$

$\eta$  being an arbitrary number. This set was found after some trials. Actually at the beginning we used the set  $\{\mathbf{e}_i, i = 1, \dots, p\}$ ,  $\mathbf{e}_i$  being the  $i$ th coordinate direction. Surprisingly, some  $\mathbf{e}_i$  proved so close to an eigenvector  $\mathbf{v}_{N-k+1}$ ,  $k > p$ , of some test matrices, that  $\mathbf{g}_i^{(0)}$  was numerically zero.

Unless otherwise specified,  $\text{NREST} = 20$  is assumed in the numerical experiments that follow.

Figure 1 shows that already for  $N = 156$  the simultaneous iteration methods SRQCG1 [16] and SRQCG2 [15] do not converge in practice, while the accelerated scheme SRQMCG2(L) achieves a very accurate solution after a few tens of iterations. Figure 1 suggests that preconditioning is fundamental to have convergence which appears to rely primarily on the quality of the preconditioner. Figures 2, 3, and 4 are similar to Fig. 1 and have been derived for  $N = 812$ , 1802, and 2304, respectively. Again we observe that the convergence rate of SRQMCG2(L) is very high, while the simultaneous algorithms without acceleration fail to work. It is to be noted that the pointwise incomplete Cholesky decomposition requires a small computational effort (as compared to a single SRQMCG2(L) iteration) and a limited amount of additional computer storage for  $\mathbf{L}$ . Superior preconditioners are more expensive in terms of both CPU time and memory requirement. Figures 1 through 4 indicate that our preconditioning is very effective regardless of the magnitude of the spectral condition number of the Hessian (see [53]) which for our test matrices achieves values of the order of  $10^{10}$  [19]. With regard to SRQMCG2(D), Figs. 3 and 4 emphasize that a simple diagonal scaling may represent a very poor preconditioning, especially if  $\mathbf{A}$  is not diagonally dominant (the matrix with  $N = 1802$  indeed is not). Note that the average residual does not decrease monotonically with  $k$  and may display significant oscillations (Fig. 4).

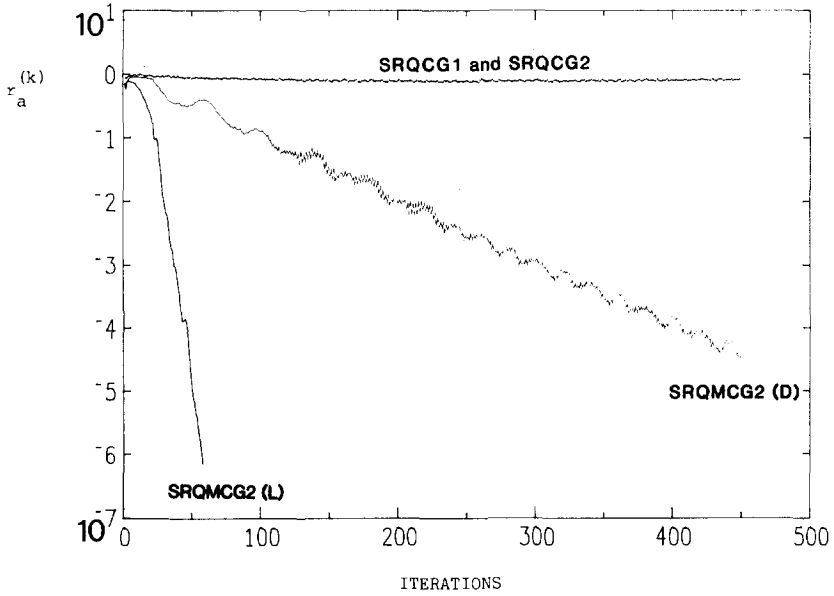


FIG. 1. Convergence profiles in the calculation of the leftmost  $p$  eigenpairs by the simultaneous iteration method with and without preconditioning ( $N=156$ ).

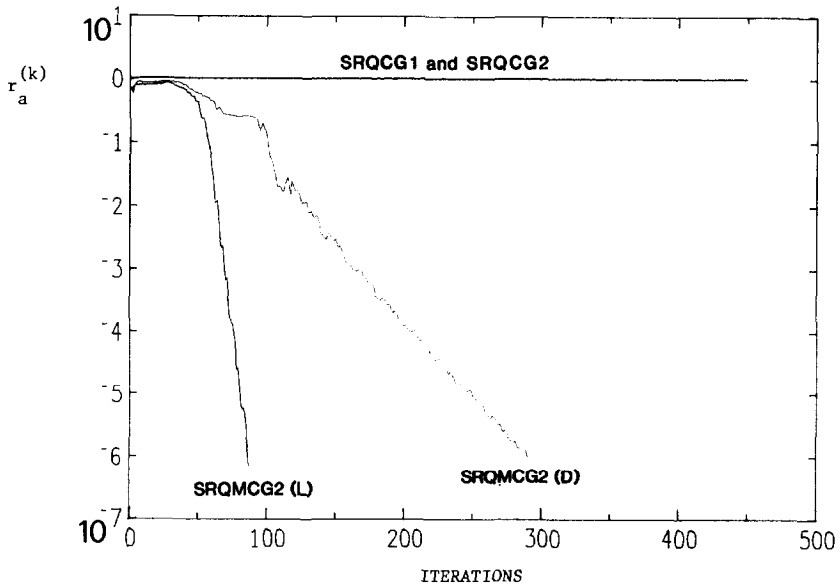
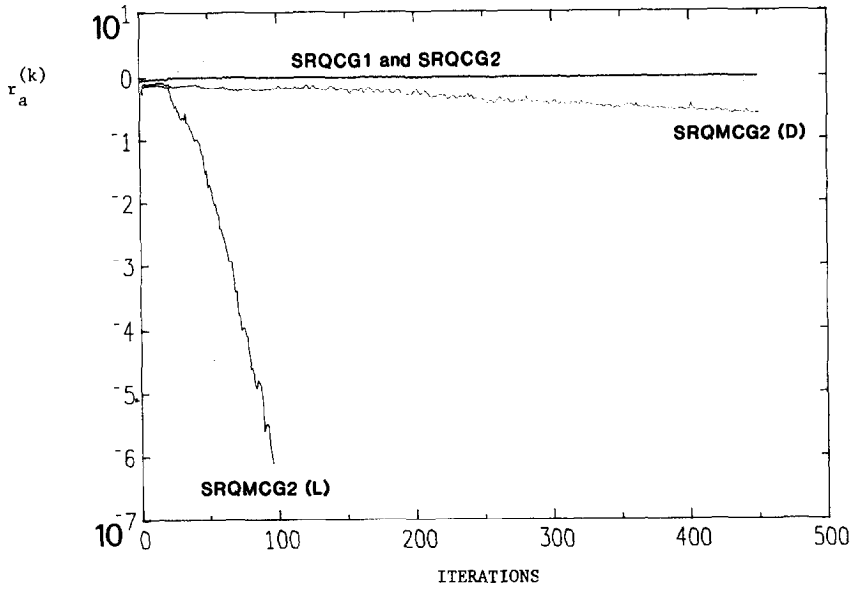
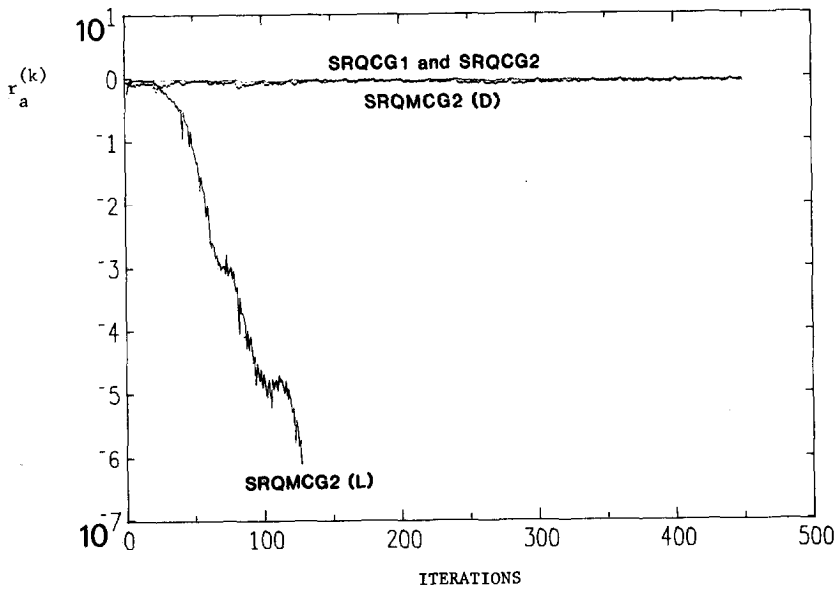


FIG. 2. The same as Fig. 1 for  $N=812$ .

FIG. 3. The same as Fig. 1 for  $N = 1802$ .FIG. 4. The same as Fig. 1 for  $N = 2304$ .

As is generally expected, the convergence rate toward  $\mathbf{v}_{N-j+1}$  decreases as the eigenpair level  $j$  increases, i.e., the leftmost eigenvectors are determined earlier. This is shown in Fig. 5 for SRQMCG2(L) and  $N = 156$ , but the profile behaviour is the same for the larger values of  $N$  as well. Figure 5 provides documentary evidence that the average convergence (profile denoted by “+”) slows down as the number  $p$  of wanted eigenpairs increases.

The influence of the restarting Ritz step on the convergence of SRQMCG2(L) is pointed out in Figs. 6 and 7, relevant to  $N = 812$  and  $N = 2304$ , respectively. It is worth observing that the accelerated simultaneous iterations fail to converge if the restarting procedure is not performed. This is so because the orthogonalization process applied to the minimization directions in the long run destroy the properties of the conjugate gradient optimization algorithm. The failure to converge has been recently pointed out also by Longsine and McCormick [15] and Schwarz [16]. However, as early as 1974 Ruhe [54] had noted that “this restart is important to insure convergence in cases needing many iterations.”

Inspection of the Figs. 6 and 7 shows that a good value of NREST is between 10 and 20. The same conclusion was arrived at when the experiments were made on the matrices with  $N = 156$  and  $N = 1802$ . The case NREST = 1 is quite peculiar: SRQMCG2(L) reduces to a preconditioned CG method combined with the Ritz projection procedure. Figures 6 and 7 show that the efficiency of this scheme is lower than that obtained using any value of NREST smaller than 50.

Figures 6 and 7 stress the importance of the restarting step to have a good

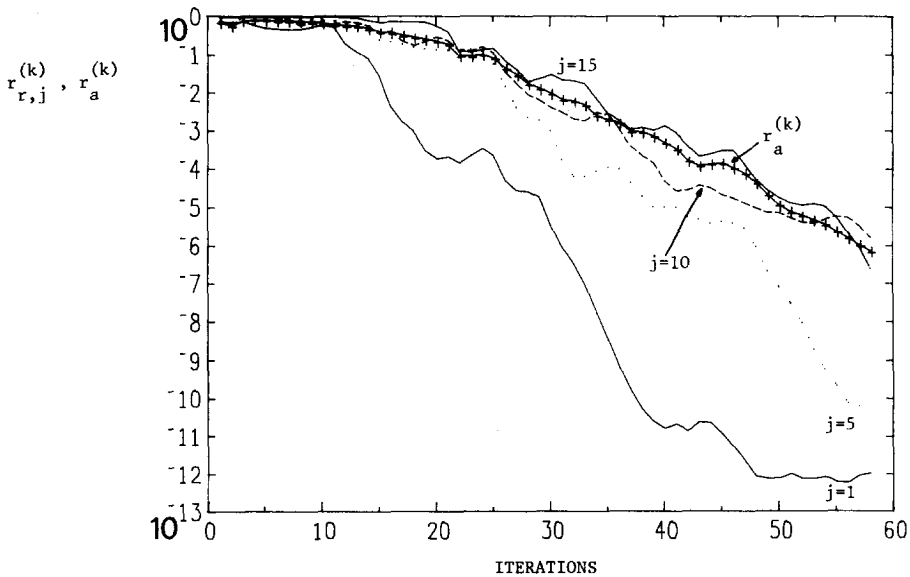


FIG. 5. Single  $[r_{r,j}^{(k)}]$  and average  $[r_a^{(k)}]$  convergence profiles in the calculation of the leftmost  $p$  eigenpairs by the accelerated simultaneous iteration scheme SRQMCG2(L) for the matrix with  $N = 156$ .

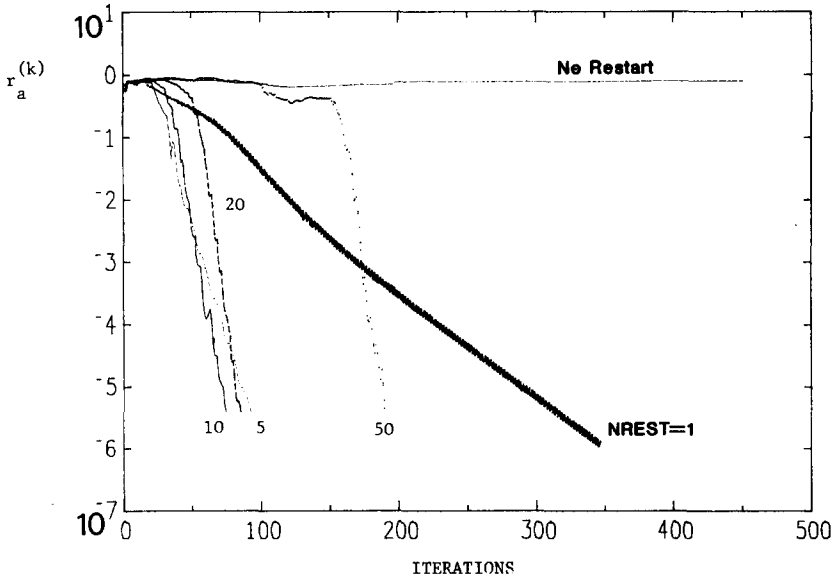


FIG. 6. Convergence profiles in the calculation of the leftmost  $p$  eigenpairs by the accelerated simultaneous iteration scheme SRQMG2(L) when a Ritz projection step is implemented in the restarting procedure, for several values of  $NREST$  ( $N = 812$ ).

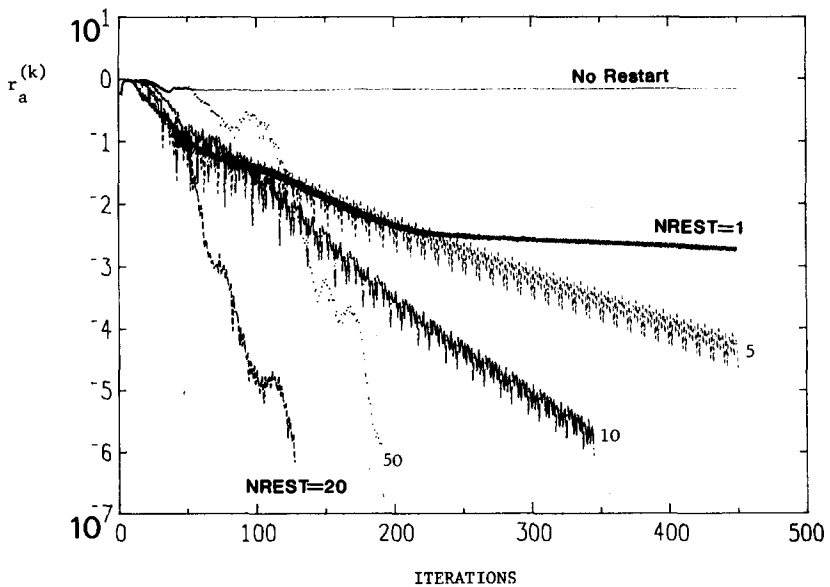


FIG. 7. The same as Fig. 6, for  $N = 2304$ .

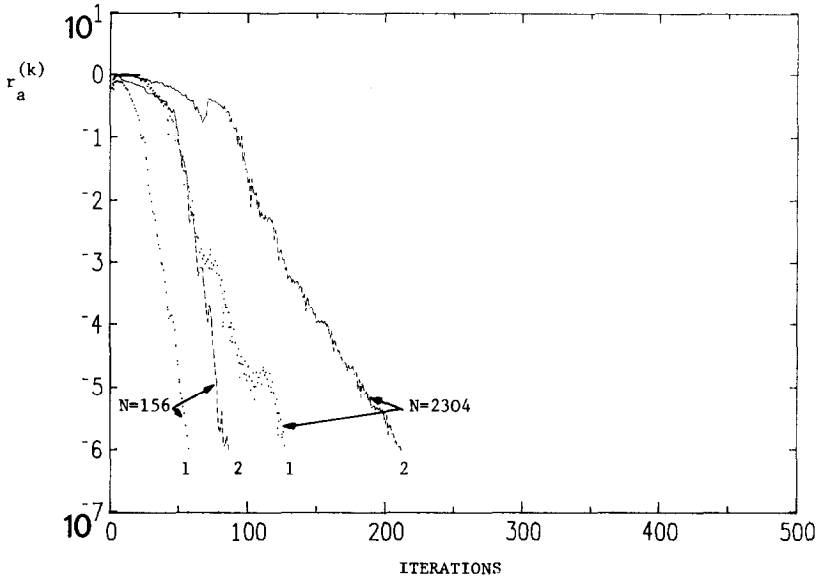


FIG. 8. Convergence profiles in the calculation of the leftmost  $p$  eigenpairs by the accelerated simultaneous iteration scheme SRQMCG2(L) with (curve 1) and without (curve 2) the implementation of the Ritz projection step in the restarting procedure (NREST = 20).

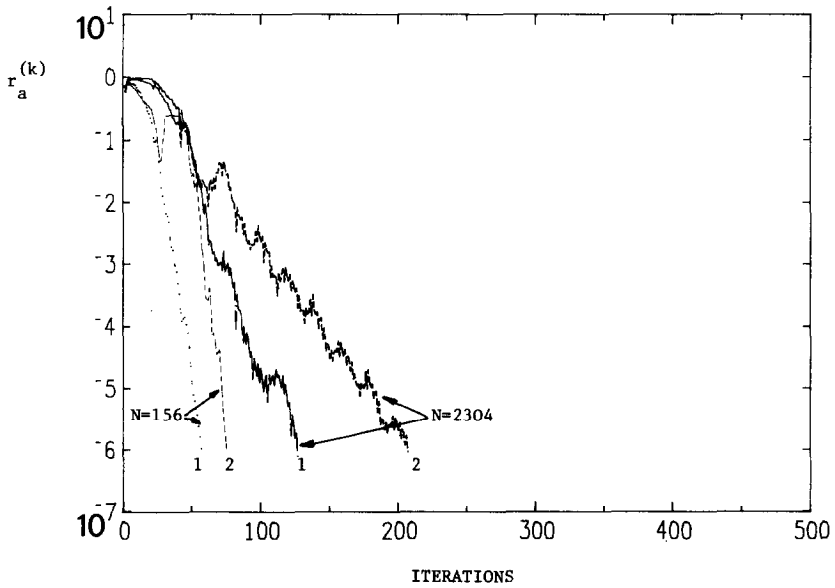


FIG. 9. Comparison between the convergence rates of SRQMCG2(L) (curves 1) and SRQMCG1(L) (curves 2) for NREST = 20. In the restarting procedure a Ritz projection step is performed.

convergence. Figure 8 shows that the simple restarting is substantially improved if the initial set  $\bar{\mathbf{X}}^{(k)}$  is the outcome from a Ritz projection step onto  $\text{span}(\mathbf{X}^{(k)})$  determined by the last current eigenvector approximations.

Finally the performances of SRQMCG1(L) and SRQMCG2(L) are compared in Fig. 9. In keeping with the results from the simultaneous scheme without acceleration, Fig. 9 emphasizes the superiority of SRQMCG2(L) to SRQMCG1(L). The former is therefore to be preferred in the simultaneous preconditioned evaluation of the leftmost eigenspectrum of large arbitrarily sparse finite element matrices.

### 3. CONCLUSIONS

The following remarks are worth summarizing.

(1) The Rayleigh quotient conjugate gradient iterations for the simultaneous computation of the leftmost  $p$  eigenpairs of symmetric positive definite problems [15, 16] do not lead to practical convergence when  $\mathbf{A}$  is a large arbitrarily sparse finite element matrix.

(2) An acceleration of the simultaneous iterations based on a preconditioning has been proposed, implemented, and numerically tested upon several finite element matrices with size between 156 and 2304. The results show that the smallest  $p$  (with  $p = 15$ ) eigenpairs are accurately determined by the preconditioned scheme after a number of iterations which is much smaller than  $N$ , and particularly so for the largest values of  $N$ .

(3) The performance of the accelerated algorithm has been explored with two different and inexpensive preconditioners. The simple diagonal scaling proved unreliable in at least two examples. By contrast the pointwise incomplete Cholesky factorization turned out to be a robust, reliable, and efficient technique of preconditioning.

(4) To have practical convergence the accelerated scheme is to be restarted after a prescribed number of iterations NREST. Convergence is improved if the current eigenvector approximations at the restart are preliminarily processed by a Ritz projection step. In all the experiments a good value for NREST was between 10 and 20. NREST close to 20 proved appropriate irrespective of the matrix size  $N$ .

(5) Two different preconditioned schemes were analysed, according to the original algorithms implemented in [15, 16]. Surprisingly enough, their behaviours were quite different. The method derived from [15] turned out to converge faster than that based on the work [16].

(6) The promising results obtained with the preconditioned iterations suggest that further improvement in the computational cost can be achieved by a suitable vectorization of the algorithms. Investigations along this direction are currently under way at the University of Padua, Italy.

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