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Spectral acceleration of parallel iterative eigensolvers for large scale scientific computing

Luca BERGAMASCHI [a,1], and Ángeles MARTÍNEZ [b]
[a] *Department of Civil Environmental and Architectural Engineering, University of Padua*
[b] *Department of Mathematics, University of Padua*

Abstract. The computation of a number of the smallest eigenvalues of large and sparse matrices is crucial in various scientific applications, as the Finite Element solution of PDES, electronic structure calculations or Laplacian of graphs, to mention a few. We propose in this contribution a parallel algorithm which is based on the spectral, low-rank, modification of a sparse inverse preconditioner (RFSAI) to accelerate Newton-based iterative eigensolvers. Numerical results onto matrices arising from various realistic problems with size up to 5 million unknowns and 2.2×10^8 nonzero elements account for the efficiency and the scalability of the proposed RFSAI–updated preconditioner.

Keywords. Eigenpairs, Newton's method, preconditioners, approximate inverses

1. Acceleration of eigensolvers by spectral preconditioners

Consider a symmetric positive definite (SPD) matrix A, which is also assumed to be large and sparse. We will denote as $0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_m \leq \ldots \leq \lambda_n$ the eigenvalues of A and $v_1, v_2, \ldots, v_m, \ldots, v_n$ the corresponding (normalized) eigenvectors.

To compute the $j-$th leftmost eigenpair we choose the DACG-Newton method [2]. The DACG solver[3], is used to assess a rough initial approximatione of the eigenvector which is refined by the subsequent projected Newton method. In this paper we propose a parallel implementation of a new preconditioning strategy as proposed in [1] for accelerating the Newton stage, namely the Newton method in the unit sphere:

$$\text{solve by PCG} \quad J_k^{(j)} s_k = -r_k; \qquad \text{Set} \quad t = u_k + s; \qquad u_{k+1} = t\|t\|^{-1}$$

$$\text{where} \quad J_k^{(j)} = (I - QQ^\top)(A - \theta_k I)(I - QQ^\top),\ r_k = Au_k - \theta_k u_k, \quad \theta_k = u_k^\top A u_k$$

$$Q = \begin{bmatrix} v_1\ v_2 \ldots v_{j-1}\ u_k \end{bmatrix}$$

The idea is to use the initial DACG approximation not only as an initial eigenvector guess for the Newton phase, but also to construct a spectral preconditioner for the efficient

[1] Corresponding Author: Luca Bergamaschi, Dept. of Civil Environmental and Architectural Engineering, University of Padua, E-mail: luca.bergamaschi@unipd.it.