Parallel solution of the generalized eigenvalue problem given in a factored form

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The standard LAPACK algorithm for the generalized Hermitian eigenproblem

$$Ax = \lambda Bx,$$

where both matrices are Hermitian, and B is positive definite, performs a reduction to the standard eigenvalue problem by using the Cholesky factorization of B. Such an approach is not well suited for the parallel computation since the Cholesky factorization is inherently sequential.

In the FLAPW Method (Full Potential Linearized Augmented Plane Wave Method) – an electronic structure method in solid state physics – the obtained generalized eigenvalue problem is of the form

$$A = \sum_{k=1}^{n} A_k^* T_k A_k, \quad B = \sum_{k=1}^{n} B_k^* B_k,$$

where T_k are Hermitian and indefinite, and the matrices A_k^* and B_k^* are tall and skinny. Instead of explicitly forming A and B, and then computing the generalized eigendecomposition, another approach is to transform the problem into an implicit generalized eigenvalue problem, i.e., into a hyperbolic generalized SVD, of the following form

$$(A, B) := (F^* J F, G^* G),$$

with F and G that have approximately three times more rows than columns, and $J = \mathrm{diag}(\pm 1)$.

We show how to modify the Hari–Zimmermann method for the generalized eigenproblem to work in parallel on A and B implicitly, i.e., not directly on the matrices A and B, but on their factors F, G, and J instead. The parallelization approach has three stages. First, the matrices T_k are factored in parallel by the Hermitian indefinite factorizations, revealing the sign matrix J. Then, the obtained factors are used to form F. Finally, the hyperbolic generalized SVD of a pair $(F^* J F, G^* G)$ is computed. As a preprocessing part of the last stage, the pair can optionally be "shortened" to the one with square matrices by the hyperbolic QR factorization of F and the ordinary QR factorization of G.

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