論文 / 著書情報
Article / Book Information

題目(和文)	ランク構造固有値問題に対する階層的QR分解とLDL分解
Title(English)	Hierarchical QR and LDL Decomposition for Rank-Structured Eigenvalue Problems
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種別(和文)	論文要旨
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論 文 要 旨

THESIS SUMMARY

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要旨（英文 800 語程度）
Thesis Summary （approx.800 English Words ）

Eigenvalue problems lie at the core of many problems in computational science and engineering. Their numerical solution plays a crucial role in many application areas, such as studying dynamics of electromagnetic fields, electronic state calculations, vibration analysis, particle accelerator and neutron flow simulations, and many more. However, traditional dense eigenvalue algorithms require a prohibitive cost of $O(n^3)$ operations. As the rapid advances in scientific computing demand solving for large matrices, fast and accurate eigenvalue algorithms are required to tackle more complex and large-scale problems.

This thesis presents two essential tools to solve the symmetric eigenvalue problems involving dense matrices with rank-deficient off-diagonal sub-blocks, which often arise from many application areas. The proposed methods utilize the structured low-rank property of such matrices through hierarchical low-rank approximation to obtain fast eigenvalue algorithms with controllable accuracy.

In the first part, two new algorithms for the QR decomposition of Block Low-Rank (BLR) matrices are presented along with their application to the QR eigenvalue algorithm, which has been the standard method to compute all eigenvalues in the dense linear algebra community. The first algorithm is based on the blocked Householder method with $O(mn)$ complexity, and the second one is based on the tiled Householder method that exhibits $O(mn^{1.5})$ complexity. The parallelization on shared memory systems is also presented. Numerical results show that the proposed algorithms are orders of magnitude faster than the state-of-the-art dense QR decomposition of Intel MKL. Moreover, the proposed method also achieves higher parallel scalability and robustness to ill-conditioning than an existing Gram-Schmidt-based BLR method. Furthermore, applying them to the QR algorithm produces a BLR-QR eigenvalue algorithm with controllable accuracy. However, its performance suffers from the growing rank of the off-diagonal blocks that happen as a result of the QR iteration. Although this suggests that the proposed BLR-QR decomposition can not be used to obtain efficient QR iteration, it can still be used for other applications, such as the tridiagonal reduction of BLR matrices, which can then be combined with many kinds of eigenvalue algorithms. In addition, the proposed BLR-QR decomposition can also be used to solve least squares problems efficiently in shared and distributed memory systems.

In the second part, the LDL decomposition of hierarchically semi-separable (HSS) and H^2 matrices, along with their application to the bisection eigenvalue algorithm, are investigated. The first algorithm extends an existing generalized LDL decomposition of HSS matrices to distributed memory systems in order to obtain a highly parallel algorithm with $O(n)$ complexity. Applying it to the bisection method results in a fast and scalable algorithm to compute the k-th smallest eigenvalue of HSS matrices in near-linear time. Numerical results show a dramatic speedup and better parallel scalability over the vendor-optimized parallel dense eigenvalue solvers in LAPACK and ScaLAPACK, efficiently utilizing tens of thousands of CPU cores across hundreds of computing nodes. This is mainly attributed to the inherent parallelism of the generalized LDL decomposition when combined with the simple structure of the HSS matrices. The second algorithm further extends the generalized LDL decomposition of HSS matrices to H^2 matrices. Although this extension leads to a reduced degree of parallelism compared to the HSS counterpart, it allows for tackling more general problem classes efficiently. Particularly, the problems originating from 3D geometries where the HSS-based method suffers from performance degradation, making it unable to attain the linear complexity that the H^2-based method achieves. This is verified by applying both methods to the bisection eigenvalue algorithm in order to solve the k-th eigenvalue problems arising from the electronic state calculations of carbon nanomaterials, which are 3D in nature. Results on a single node show that the H^2-based bisection method outperforms the existing HSS-based method due to the HSS compression rank that grows proportionally

with the matrix size. Comparison between the two methods on multiple nodes will be addressed in future work due to the need for distributed memory runtime system to fully exploit the parallelism of the H^2-based method. In addition, the backward error bound for the generalized LDL decomposition of H^2 matrices, which is not available at the moment, should be addressed too in order to improve its reliability.