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Parallel diagonalization performance on high-performance computers. (English)

Zbl 1183.68113

Čiegis, Raimondas (ed.) et al., Parallel scientific computing and optimization. Advances and applications. New York, NY: Springer (ISBN 978-0-387-09706-0/hbk). Springer Optimization and Its Applications 27, 57-66 (2009).

Summary: Eigenvalue and eigenvector computations arise in a wide range of scientific and engineering applications. For example, in quantum chemistry and atomic physics, the computation of eigenvalues is often required to obtain electronic energy states. For large-scale complex systems in such areas, the eigensolver calculation usually represents a huge computational challenge. It is therefore imperative that suitable, highly efficient eigensolver methods are used in order to facilitate the solution of the most demanding scientific problems. This presentation analyzes the performance of parallel eigensolvers from numerical libraries such as ScaLAPACK on the latest parallel architectures using data sets derived from large-scale scientific applications.

For the entire collection see [Zbl 1151.65001].

MSC:

68M20 Performance evaluation, queueing, and scheduling in the context of computer systems
68W30 Symbolic computation and algebraic computation

Keywords:

parallel eigensolvers; ScaLAPACK

Software:

PRMAT; ScaLAPACK

Full Text: DOI