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Rokko: Integrated interfaces for dense and sparse parallel eigensolvers

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Recently, a number of state-of-the-art hybrid parallel eigensolver libraries have been developed: EigenExa and ELPA for dense matrices, and Anasazi and SLEPc for sparse matrices, and so on. However, there are yet only a few application programs that use these solvers. This is partially due to the different function interfaces for each solver. Also, different compile and link procedures for different languages C++ / C / Fortran and different machine environments as well as the complicated dependencies on lower level libraries often become barriers of introducing new solver libraries. To overcome these difficulties, we have developed a bundle of integrated interfaces, "Rokko," which covers all the eigensolver libraries on an equal footing. Rokko allows users to select a solver at run-time by adopting the factory method. This feature enables users to readily take a benchmark of all the solvers to determine the optimal solver for the matrices used in their application programs and for their machine environment. In addition, to resolve the compile and link problems, we provide a build system which automatically detects solver libraries based on CMake utility program. Although the primary interfaces provided by Rokko are for the C++ language, we also provide the C / Fortran bindings. We illustrate simplicity of using Rokko through code fragments. We also present the results of diagonalization benchmark tests of the minij matrix and lattice Hamiltonian matrix for the antiferromagnetic quantum Heisenberg model to demonstrate the small overhead in the Rokko interfaces.

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