Eigenvalue Solvers—The ELPA Project and Beyond

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Eigenvalue and eigenvector computations are at the core of electronic structure simulations, and often they take a considerable amount of the overall time, in particular in highly parallel environments. One reason for this is the fact that the popular ScaLAPACK symmetric eigensolver does not scale well beyond one thousand cores, which is mainly due to the large number of memory accesses and the communication required by the two-sided transformations in the reduction phase.

We report on results from the ELPA project (*Eigenvalue Solvers for Petaflop Applications*) [1] that led to improved eigensolvers for dense symmetric problems, reducing administrative and communication overhead in existing algorithms, providing additional algorithmic paths (two-stage reduction to tridiagonal form and corresponding back transformation of the eigenvectors, divide-and-conquer algorithm and MRRR algorithm for partial eigensystems of symmetric tridiagonal matrices), and optimized computational kernels.

These routines provide significant speedup over the ScaLAPACK library, in particular if a large number of cores is used for moderately-sized matrices, and scalability has been demonstrated up to very large systems ($\sim$ 300k cores) [2].

We also briefly comment on further developments for matrices with particular structures.

[1] `http://elpa.rzg.mpg.de`

[2] R. Johanni et al., Scaling of eigenvalue solver dominated simulations, in TR FZJ-JSC-IB-2011-02, pp. 27–30, April 2011