clique: a Parallel Tool for the Molecular Nanomagnets Simulation and Modelling

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A powerful program for modelling the molecular nanomagnets is presented. The exact diagonalization method is used, which gives numerically accurate results. Its main bottleneck is the diagonalization time of large matrices, however it is removed by exploiting the symmetry of the compounds and implementing the method in the parallel computing environment. The diagonalization scheduling algorithm is implemented to increase the balance of the parallel processes workload. The running times of two different diagonalization procedures are compared.

Keywords: molecular nanomagnets, exact diagonalization, high performance computing.