

EFFICIENT COMPUTATION OF SPARSE MATRIX FUNCTIONS FOR LARGE-SCALE ELECTRONIC STRUCTURE CALCULATIONS: THE CHESS LIBRARY

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In this talk I will present CheSS, the “Chebyshev Sparse Solvers” library, which has been designed to solve typical problems arising in large-scale electronic structure calculations using localized basis sets. The library is based on a flexible and efficient expansion in terms of Chebyshev polynomials and is able to exploit the sparsity of the matrices, scaling linearly with respect to the number of nonzero entries. The approach is particularly adapted for setups leading to small spectral widths of the involved matrices and outperforms alternative methods in this regime. In addition, the approach based on Chebyshev polynomials can be massively parallelized, and CheSS exhibits excellent scaling up to thousands of cores even for relatively small matrix sizes.