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Parallel on-the-fly configuration-interaction shell-model code

WILLIAM ORMAND, Lawrence Livermore National Laboratory, CALVIN JOHNSON, PLAMEN KRASSTEV, San Diego State University — Configuration-interaction shell-model codes generally rely on computing and storing the full many-body Hamiltonian matrix, which while sparse, nonetheless push computational memory demands, especially when the number of basis states approach 10^8 and up. On-the-fly algorithms mitigate the memory burden by factorizing both the basis and the Hamiltonian. We describe BIGSTICK, an efficient on-the-fly code designed for large-scale parallel operation with both two- and three-body interactions. We present algorithm developments utilizing MPI, OPENMP, and hybrid schemes. Prepared by LLNL under Contract DE-AC52-07NA27344. Support from U.S. DOE/SC/NP (Work Proposal No. SCW0498) and U.S. DOE Grants DE-FG02-03ER41272 and DE-FC02-09ER41587 is acknowledged.

William Ormand
Lawrence Livermore National Laboratory

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