Abstract Submitted
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Data compression algorithms for electronic wave functions WILLIAM DAWSON, FRANCOIS GYGI, Univ of California - Davis — Large scale, First-Principles Molecular Dynamics (FMPD) simulations require an large amount of computational effort. Unfortunately, the size of the data they generate and the overhead cost of saving it result in the overwhelming majority of this potentially valuable data being lost. The rising gap between CPU and file I/O performance will restrict even further the amount of data saved during future FPMD simulations. The Recursive Subspace Bisection method for generating localized wavefunctions has recently been utilized to reduce the cost of computing Hartree-Fock exchange with controlled accuracy. We show that a variation of this method can be used to compress FPMD simulation data. Furthermore, we show that this method has controlled and predictable accuracy, and can be applied without concern for specific system properties. We demonstrate this method by compressing data from the simulation of liquid water, melting silicon, and other representative systems. Supported by: DE-SC0008938.

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