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An accurate and scalable O(N) algorithm for First-Principles Molecular Dynamics computations on petascale computers and beyond[1]

DANIEL OSEI-KUFFUOR, JEAN-LUC FATTEBERT, Lawrence Livermore National Laboratory — We present a truly scalable First-Principles Molecular Dynamics algorithm with O(N) complexity and fully controllable accuracy, capable of simulating systems of sizes that were previously impossible with this degree of accuracy. By avoiding global communication, we have extended W. Kohn's condensed matter "nearsightedness" principle to a practical computational scheme capable of extreme scalability. Accuracy is controlled by the mesh spacing of the finite difference discretization, the size of the localization regions in which the electronic wavefunctions are confined, and a cutoff beyond which the components of the overlap matrix can be omitted when computing selected elements of its inverse. We demonstrate the algorithm's excellent parallel scaling for up to 100,000 atoms on 100,000 processors, with a wall-clock time of the order of one minute per molecular dynamics time step.

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