

# Large-Scale First-Principles Simulations

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## Abstract

First-principles molecular dynamics (FPMD) is emerging as a very powerful atomistic simulation approach, which combines a classical description of nuclei with a quantum mechanical description of electrons. Recent advances in electronic structure methods, notably Density Functional Theory (DFT), have made FPMD a truly predictive approach, which provides information on the structural, dynamical and electronic properties of a physical system. FPMD has been successfully applied to several areas of research in materials science, chemistry and biochemistry. The computational cost of FPMD simulations is high, due to the detailed description of electronic structure that is required. Straightforward implementations of FPMD incur a computational cost of  $O(N^3)$  for  $N$  atoms. More recent approaches have been proposed to reduce this cost to  $O(N)$ . We will present recent progress in the development of  $O(N)$  algorithms based on real-space, finite-difference methods, as well as the challenges that arise when implementing conventional  $O(N^3)$  FPMD on large, massively parallel computers.