Electronic Structure and First Principles Dynamics on Graphical Processing Units

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Massively parallel processors that can perform more than a hundred arithmetic operations per clock cycle, such as graphical processing units (GPU), have recently become mainstream in the era of petascale computing. However, in addition to the remarkable performance, these architectures posses certain limitations, such as imbalanced performance of single and double arithmetic operations and high sensitivity to various strategies for code optimization. We discuss how precision can be effectively controlled in ground state (HF, DFT) and excited state (CIS, TD-DFT) molecular dynamics by splitting the entire calculation into single precision and double precision parts, providing double precision quality results almost at the speed of purely single precision arithmetic. Using our newly developed TeraChem program, we discuss results from *ab initio* molecular dynamics calculations of solvated proteins with up to 1000 atoms. We show that charge transfer effects are not negligible and comment on the implications for simulations using empirical force fields. If time permits, we also present results for excited states of photoactive proteins using CIS and TDDFT methods, where the entire protein is modeled with *ab initio* quantum chemistry.