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GPU implementation of Car-Parrinello molecular dynamics calculations[1] JACOB H. MINER, University of Washington, ROB FARBER, Pacific Northwest National Laboratory, JOHN J. REHR, University of Washington — General Purpose Graphics Processing Units (GPUs) have great potential for speeding up scientific computing applications. With modern cards offering over one teraFLOP performance and the increasing availability of libraries and compilers, the utilization of these tools is spreading rapidly. Here we investigate how the increased computational power of GPUs makes it possible to include efficiently both nuclear and electronic degrees of freedom in complex systems. We demonstrate the speed gains and the scaling with system size of the CPMD code on GPUs, compared to conventional CPU-based computer systems on several examples. We also discuss some of the challenges in implementing GPUs on these codes.

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