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GPU Acceleration of the Qbox First-Principles Molecular Dynamics Code[1] WILLIAM DAWSON, FRANCOIS GYGI, Department of Computer Science, University of California Davis, Davis CA 95616 — The availability of double precision graphics cards provides an opportunity to speed up electronic structure computations. We modify the Qbox [1] code to utilize Fermi GPUs on the Keeneland [2] platform. We use the CUFFT library to speed up Fourier transforms and perform asynchronous communication to cut down the cost of data transfers. The modified code is used in simulations of a 64-molecule water system with an 85 Ry plane wave energy cut off. Preliminary results show a 2-3 times speedup in the calculation of the charge density and in the application of the Hamiltonian operator to the wave function. We present these findings as well as further speedups measured in other parts of the code.

[1] http://eslab.ucdavis.edu/software/qbox
[2] http://keeneland.gatech.edu

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