Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

A scalable algorithm for the computation of Hartree-Fock exchange[1] IVAN DUCHEMIN, FRANCOIS GYGI, University of California Davis, Davis CA 95616 — Electronic structure calculations based on hybrid density functionals require efficient algorithms for the computation of the Hartree-Fock exchange operator. The high computational cost of Hartree-Fock exchange currently limits the use of such functionals in large-scale First-Principles Molecular Dynamics applications. We present a scalable parallel algorithm for the computation of Hartree-Fock exchange in a plane-wave, pseudopotential framework, with applications to electronic structure calculations of liquid water and various nanostructures. Technical issues arising in the implementation of hybrid density functionals will be discussed.

[1]Supported by NSF OCI 0749219 and DOE-SciDAC DE-FC02-06ER25794

Francois Gygi
University of California Davis, Davis CA 95616

Date submitted: 20 Nov 2008 Electronic form version 1.4