

Abstract Submitted  
for the MAR17 Meeting of  
The American Physical Society

**Hybrid Grid and Basis Set Approach to Quantum Chemistry DMRG**<sup>1</sup> EDWIN MILES STOUDENMIRE, STEVEN WHITE, Univ of California - Irvine — We present a new approach for using DMRG for quantum chemistry that combines the advantages of a basis set with that of a grid approximation. Because DMRG scales linearly for quasi-one-dimensional systems, it is feasible to approximate the continuum with a fine grid in one direction while using a standard basis set approach for the transverse directions. Compared to standard basis set methods, we reach larger systems and achieve better scaling when approaching the basis set limit. The flexibility and reduced costs of our approach even make it feasible to incorporate advanced DMRG techniques such as simulating real-time dynamics.

<sup>1</sup>Supported by the Simons Collaboration on the Many-Electron Problem

Edwin Miles Stoudenmire  
Univ of California - Irvine

Date submitted: 10 Nov 2016

Electronic form version 1.4